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ENVIRO
Technical
Information for
Problem
Spills

2 - ETHYLHEXANOL

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ENVIRONMENTAL AND TECHNICAL INFORMATION FOR PROBLEM SPILLS MANUALS

Environmental and Technical Information for Problem Spills (EnviroTIPS) manuals provide detailed information on chemical substances. This information is intended to assist the reader in designing countermeasures for spills and to assess their impact on the environment. The manual has been reviewed by the Technical Services Branch, Environmental Protection Service, and approved for publication. Approval does not necessarily signify that the contents reflect the views and policies of the Environmental Protection Service. Mention of trade names or commercial products does not constitute endorsement for use.

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2-ETHYLHEXANOL

ENVIRONMENTAL AND TECHNICAL INFORMATION FOR PROBLEM SPILLS

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Environmental Protection Programs Directorate
Environmental Protection Service
Ottawa, Ontario

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FOREWORD

The Environmental and Technical Information for Problem Spills (EnviroTIPS) manuals were initiated in 1981 to provide comprehensive information on chemicals that are spilled frequently in Canada. The manuals are intended to be used by spill specialists for designing countermeasures for spills and to assess their effects on the environment. The major focus of EnviroTIPS manuals is environmental. The manuals are not intended to be used by first-response personnel because of the length and technical content; a number of manuals intended for first-response use are available. The information presented in this manual was largely obtained from literature review. Efforts were made, both in compilation and in review, to ensure that the information is as correct as possible. Publication of these data does not signify that they are recommended by the Government of Canada, nor by any other group.

ACKNOWLEDGEMENTS

The final version of this manual was prepared by the staff of the Environmental Protection Service who wrote extensive revisions to the text, drafted illustrations and incorporated all comments and additions.

The level of detail present was made possible by the many individuals, organizations and associations who provided technical data and comments throughout the compilation and subsequent review. The draft of this manual was prepared under contract to Environment Canada by M.M. Dillon Consulting Engineers and Planners, Concord Scientific Corporation, and Waterloo Engineering Limited.

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1 SUMMARY

2-ETHYLHEXANOL ($C_8H_{18}O$)

Clear, colourless oily liquid, with an unpleasant, musty odour

SYNONYMS

2-EH, 2-ethyl hexyl alcohol, iso-octyl alcohol, 2-ethyl-1-hexanol

IDENTIFICATION NUMBERS

UN No. 1987; CAS No. 104-76-7; STCC No. Not required

GRADES & PURITIES

Technical: 99.5 to 99.9 percent purity

IMMEDIATE CONCERNS

Fire: Combustible

Human Health: Low toxicity by all routes

Environmental: Harmful to aquatic life at concentrations as low as 10 ppm

PHYSICAL PROPERTY DATA

State (15°C, 1 atm): liquid
Boiling Point: 182-186°C
Melting Point: -70°C
Flammability: combustible
Flash Point: 73°C (CC)
Specific Gravity (water = 1): 0.833 @ (20°/4°C)
Solubility (in water): 0.1 g/100 mL (20°C)
Behaviour (in water): floats, with no reaction
Behaviour (in air): evaporates slowly
Odour Threshold Range: 0.08 - 0.14 ppm

ENVIRONMENTAL CONCERNS

2-Ethylhexanol has not been found to have any food chain concentration potential.

HUMAN HEALTH

No TLV or IDLH established.

Exposure Effects

Inhalation: Inhalation toxicity hazard is low, unless the material is heated or misted. Exposure to vapours can produce eye, nasal, and lung irritation

Contact: Material is absorbed fairly readily through the skin and can cause sensitization and dermatitis on prolonged or repeated contact. Eye contact causes irritation

IMMEDIATE ACTION

Spill Control

Restrict access to spill site. Issue warning: "COMBUSTIBLE". Call fire department and notify manufacturer. Eliminate sources of ignition including traffic and equipment. Stop the flow and contain spill, if safe to do so. Avoid contact. Keep contaminated water from entering sewers or watercourses.

Fire Control

Use foam, dry chemical, carbon dioxide or water fog to extinguish. Cool fire-exposed containers with water. Stay clear of tank ends.

COUNTERMEASURES

Emergency Control Procedures in/on

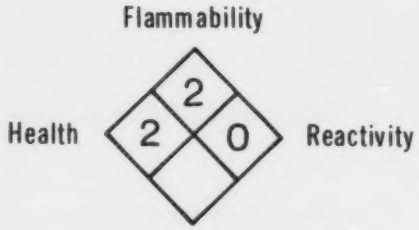
Soil: Construct barriers to contain spill. Remove material with pumps or vacuum equipment. Absorb small amounts of spill with sorbents

Water: Contain with booms. Use (oil) skimming equipment to remove slick, followed by the application of sorbents

NAS HAZARD RATING

Category	Rating
Fire	1
Health	
Vapour Irritant	1
Liquid or Solid Irritant	1
Poison	1
Water Pollution	
Human Toxicity	1
Aquatic Toxicity	1
Aesthetic Effect	2
Reactivity	
Other Chemicals	2
Water	0
Self-reaction	0

NFPA
HAZARD
CLASSIFICATION



2 PHYSICAL AND CHEMICAL DATA

Physical State Properties

Appearance	Clear, colourless liquid (BASF PSDS 1981)
Usual shipping state(s)	Liquid (BASF PSDS 1981)
Physical state at 15°C, 1 atm	Liquid
Melting point	-70°C (Kirk-Othmer 1978; ISH 1977)
Boiling point	182-186°C (Eastman 1977; Kirk-Othmer 1978; Ullmann 1975)
Vapour pressure	0.03 kPa (20°C) (PB 216658)

Densities

Specific gravity	0.8328 (20°/4°C) (CRC 1980) 0.834 (20°/20°C) (Kirk-Othmer 1978)
Vapour density	4.49 (Verschueren 1977)

Fire Properties

Flammability	Combustible liquid (NFPA 1978)
Flash point CC OC	73°C (NFPA 1978) 85°C (CHRIS 1978) 82-84°C (Kirk-Othmer 1978; Eastman 1977)
Autoignition temperature	231°C (NFPA 1978) 288°C (Eastman 1977)
Burning rate	4.0 mm/min (CHRIS 1978)
Upper flammability limit	9.7 percent (v/v) (NFPA 1978)
Lower flammability limit	0.88 percent (v/v) (NFPA 1978)
Heat of combustion	5287.8 kJ/mole (25°C) (Sussex 1977)
Combustion products	Carbon dioxide and water
Flashback potential	Very low (BASF 1982)
Electrical ignition hazard	May be ignited by a static discharge

Other Properties

Molecular weight of pure substance	130.23 (CRC 1980)
Constituent components of typical commercial grade	99.5-99.9 percent 2-ethylhexanol (BASF 1982; Kirk-Othmer 1978)
Refractive index	1.4328 (20°C) (CRC 1980) 1.4392 (20°C) (Eastman 1977)

Viscosity	9.6-9.8 mPa•s (BASF PSDS 1981) 9.8 mPa•s (Kirk-Othmer 1978)
Liquid interfacial tension with air	27.6 mN/m (20°C) (CHRIS 1978) 30.0 mN/m (20°C) (ISH 1977)
Liquid interfacial tension with water	22 mN/m (22.7°C) (CHRIS 1978)
Latent heat of vaporization	67.4 kJ/mole (25°C) (Sussex 1977)
Heat of formation	-432.8 kJ/mole (25°C) (Sussex 1977)
Heat capacity	
constant pressure (Cp)	2.36 J/(g•°C) (20°C) (ISH 1977)
Ionization potential (est.)	9.7 eV (Holmes 1981)
Critical pressure	3526 kPa (CHRIS 1978)
Critical temperature	377°C (CHRIS 1978)
Coefficient of thermal expansion	8.519 x 10^{-4}/°C (20°C) (BASF 1982) 8.75 x 10^{-4}/°C (up to 20°C), 4.02 x 10^{-4}/°C (up to 55°C) (ISH 1977)
Log_{10} octanol/water partition coefficient	3.15 (Hansch and Leo 1979)
Solubility	
In water	0.1 g/100 mL (20°C) (BASF PSDS 1981) (solubility of water in 2-ethylhexanol is 2.6 percent by weight (20°C) (Kirk-Othmer 1978))
In other common materials	Soluble in ethanol, diethyl ether, acetone and benzene (CRC 1980)

Vapour Volume Conversion

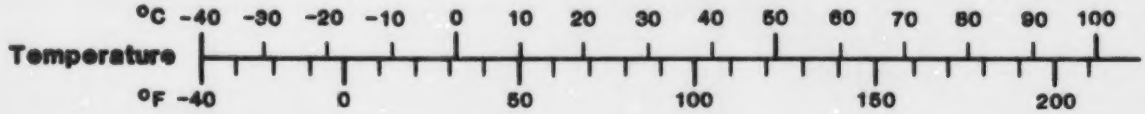
1 mg/m^3 = 0.18 ppm

1 ppm = 5.41 mg/m^3 (20°C) (Verschueren 1977)

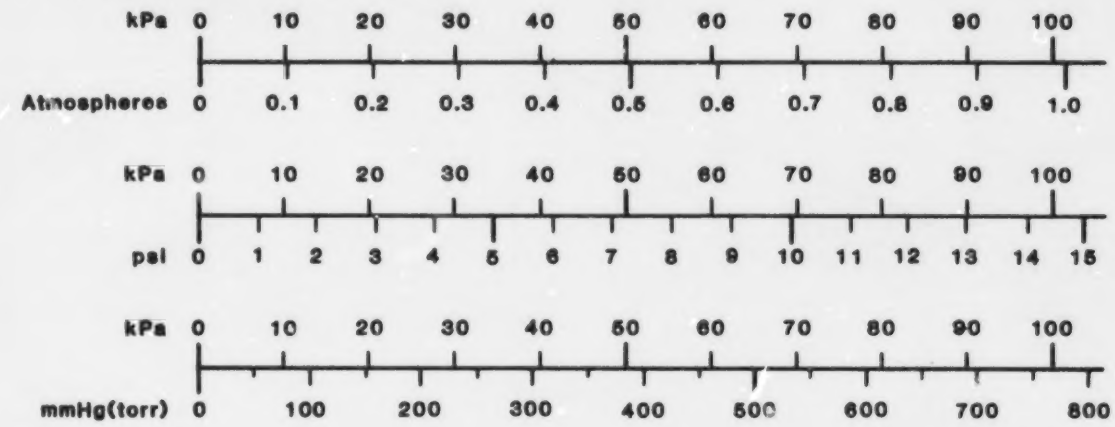
TABLE 1

2-ETHYLHEXANOL

CONVERSION NOMOGRAMS



Pressure 1 kPa = 1,000 Pa



Viscosity

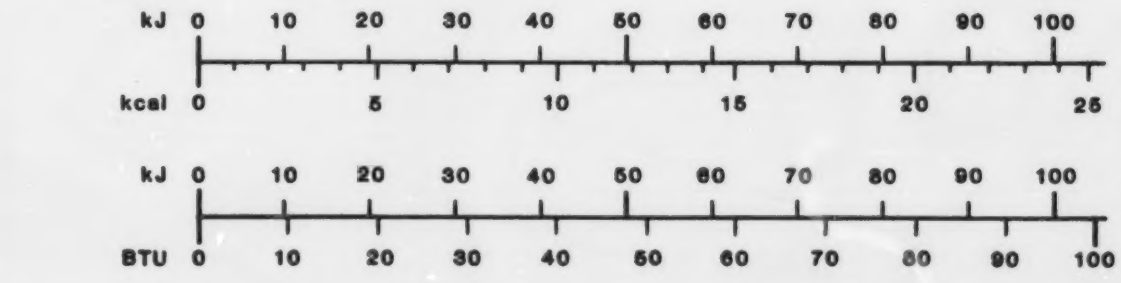
Dynamic 1 Pa·s = 1 000 centipoise (cP)

Kinematic 1 m^2/s = 1 000 000 centistokes (cSt)

Concentration (in water)

1 ppm ≅ 1 mg/L

Energy (heat) 1 kJ = 1,000 J



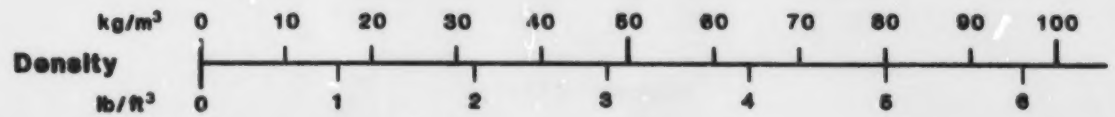


FIGURE 1

2-ETHYLHEXANOL

VAPOUR PRESSURE vs TEMPERATURE

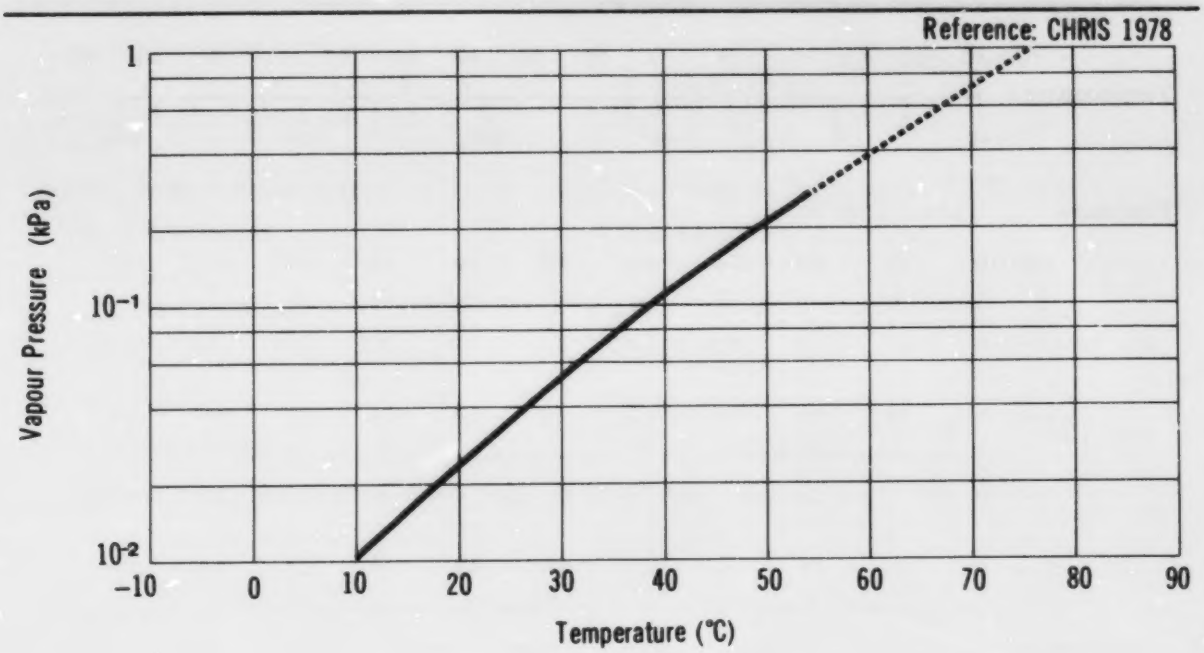


FIGURE 2

2-ETHYLHEXANOL

SATURATED VAPOUR DENSITY vs TEMPERATURE

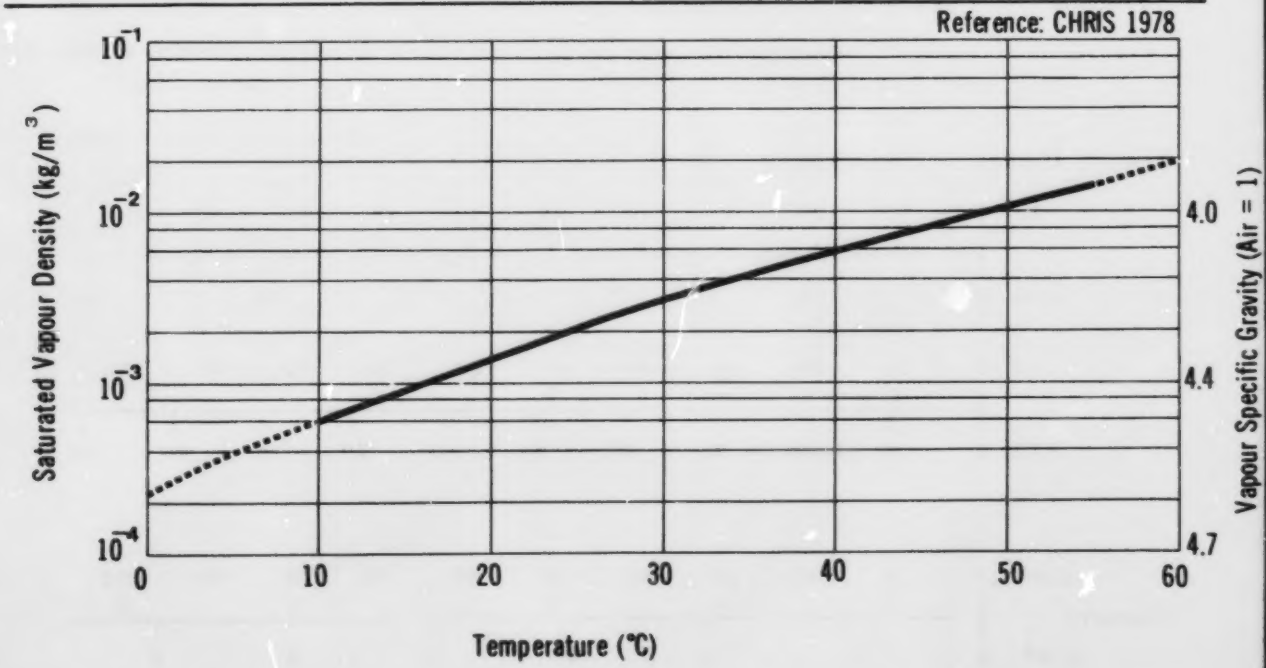


FIGURE 3

2-ETHYLHEXANOL

LIQUID DENSITY vs TEMPERATURE

Reference: CHRIS 1978

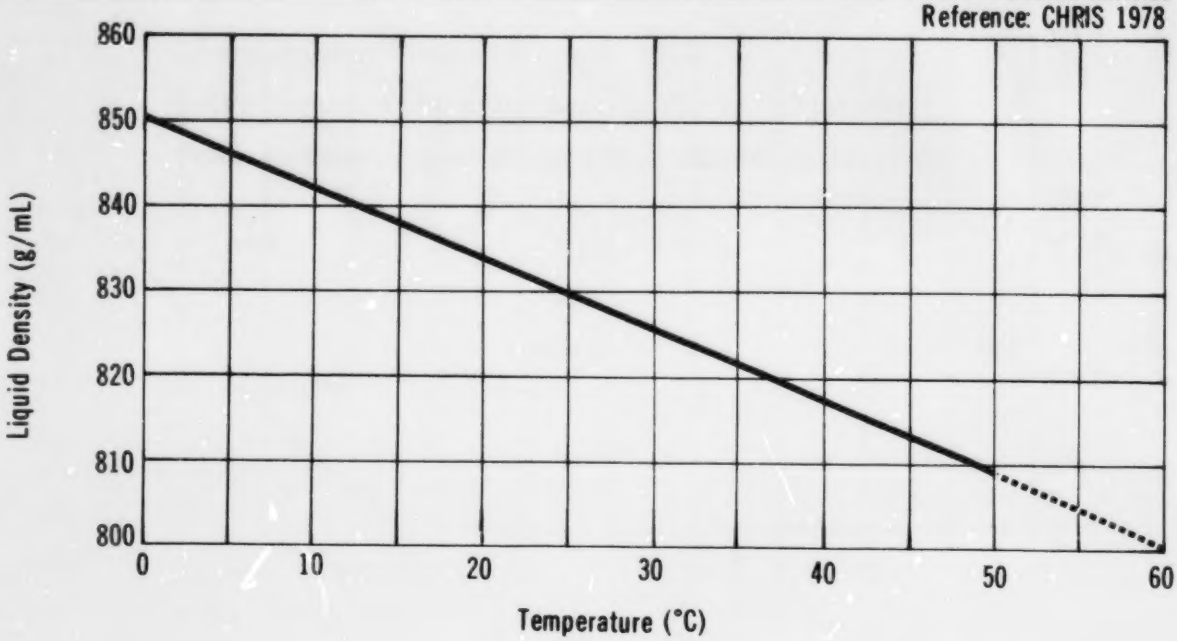


FIGURE 4

2-ETHYLHEXANOL

LIQUID VISCOSITY vs TEMPERATURE

Reference: CHRIS 1978

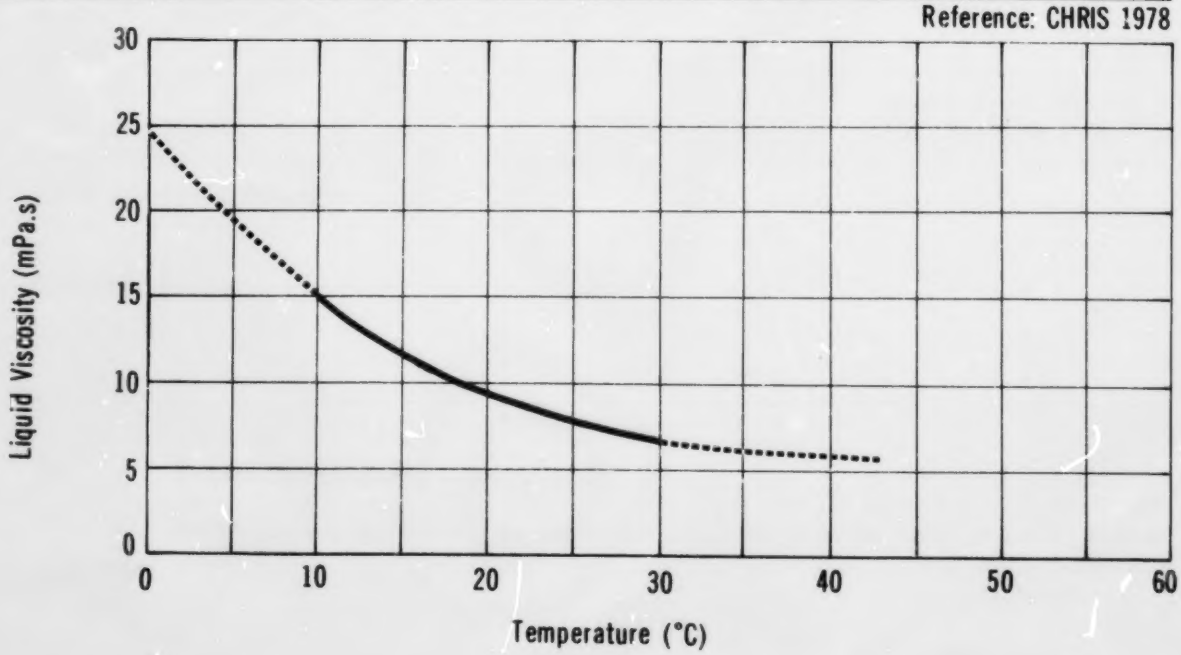
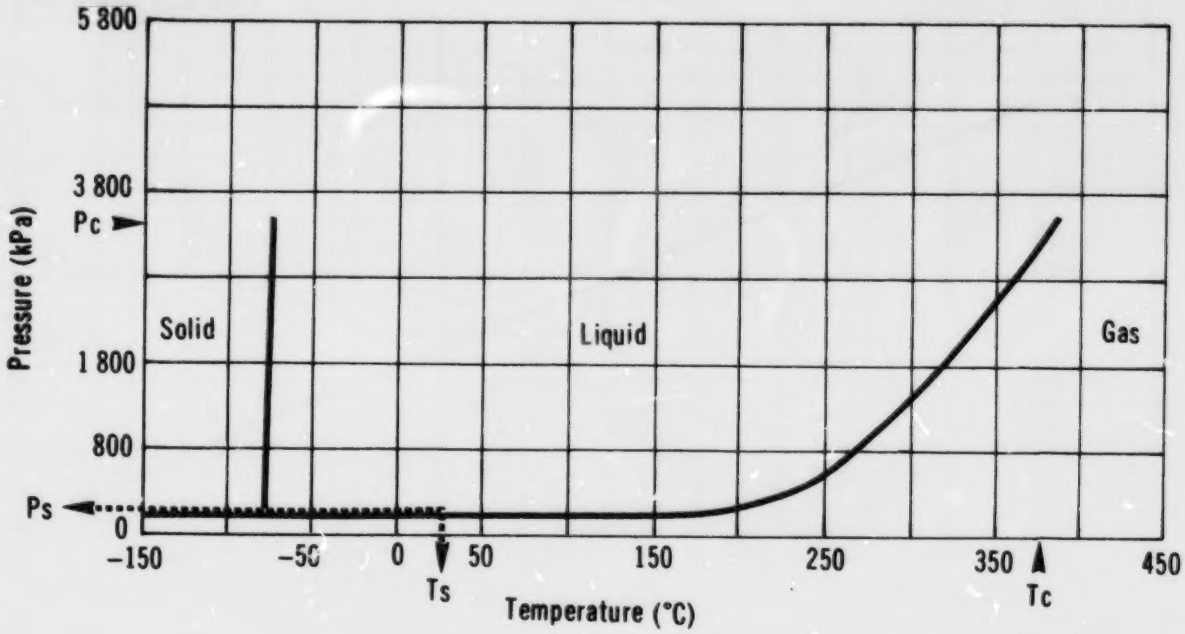


FIGURE 5

2–ETHYLHEXANOL

PHASE DIAGRAM



3 COMMERCE AND PRODUCTION

3.1 Grades, Purities (Corpus 1983; BASF 1982)

2-Ethylhexanol is sold with a purity of 99.5 to 99.9 percent.

3.2 Domestic Manufacturer (Corpus 1983; CBG 1980; BASF 1982)

BASF Canada Inc.
5850 Cote de Liesse
Montreal, Quebec
H4T 1C1
(514) 341-5411

3.3 Other Supplier (Corpus 1983)

Bate Chemical Co. Ltd.
160 Lesmill Road
Don Mills, Ontario
M3B 2T7
(416) 445-7050

3.4 Major Transportation Routes

Current Canadian production of 2-ethylhexanol is located in Laval, Quebec. The market area is mainly in Ontario and Quebec, with a small amount in the western provinces.

3.5 Production Levels (Corpus 1983)

Company, Plant Location		Nameplate Capacity kilotonnes/yr (1982)
BASF Canada, Laval, Que.		59
	TOTAL	59
Domestic Production (1982)		41.0
Imports (1982)		0.3
	TOTAL SUPPLY	41.3

3.6 Future Development (Corpus 1983)

BASF Canada is planning an expansion of its world-scale plant, at Laval, in the mid-1980s.

3.7 Manufacture of 2-Ethylhexanol (FKC 1975; Kirk-Othmer 1978)

3.7.1 General. To produce 2-ethylhexanol, propylene is combined with synthesis gas (equimolar carbon monoxide and hydrogen) to form butyraldhyde; the latter undergoes an aldol condensation to produce 2-ethylhexanol.

3.7.2 Production Process. A mixture of propylene and synthesis gas is fed to an "oxo reactor". The materials react exothermically in the liquid phase, in the presence of a cobalt catalyst at 20 000 to 30 000 kPa and 120 to 150°C:

$$CH_3CH{=}CH_2 + CO + H_2 \rightarrow \underset{\text{(n-butyraldehyde) (4 parts)}}{CH_3CH_2CH_2CHO} + \underset{\text{(iso-butyraldehyde) (1 part)}}{CH_3CH(CHO)CH_3}$$

Yield is about 77 percent butyraldehydes. Reactant gases are separated by flash distillation from the reaction product, which is then hydrogenated at 150°C to 230°C and 5000 to 20 000 kPa over a nickel catalyst:

$$2CH_3CH_2CH_2CHO + H_2 \rightarrow \underset{\text{(2-ethylhexanol, 93 percent)}}{CH_3(CH_2)_3CH(C_2H_5)CH_2OH} + \text{(by-product)}\ \underset{\text{(isobutanol)}}{CH_3CH(CH_2OH)CH_3}$$

The alcohols are separated by distillation.

3.8 Major Uses in Canada (Corpus 1983; BASF 1982)

2-Ethylhexanol is used in the production of plasticizers, dioctyl phthalate, dioctyl adipate, dioctyl azelate, and trioctyl trimellitate. It is also used as a solvent in lacquers and in the textile industry. In 1982, 67 percent of domestic production was exported, and 22 percent was used for the production of dioctylphthalate.

3.9 Major Buyers in Canada (Corpus 1983; CBG 1980)

Alchem, Burlington, Ont.
Alkahl Chemicals, Mississauga, Ont.
Almatex, London, Ont.
Ashland Chemical, Mississauga, Ont.
Atkemix, Brantford, Ont.
Bate Chemical, Toronto, Ont.
Canadian General Electric, Toronto, Ont.
Carlew Chemicals, St-Remi, Que.
Cisco, Toronto, Ont.
Coté Chemicals, Chateauguay, Que.
Harrisons & Crosfield, Toronto, Ont.
International Chemical, Brampton, Ont.
Kingsley & Keith, Etobicoke, Ont.

Monsanto Canada, LaSalle, Que.
Recochem, Montreal, Que.
Rohm & Haas Canada, Toronto, Ont.
Uniroyal Chemical, Edmonton, Alta.
Van Waters & Rogers, Vancouver, B.C.

4 MATERIAL HANDLING AND COMPATIBILITY

4.1 Containers and Transportation Vessels

4.1.1 Bulk Shipment. Transportation vessels and containers under this category have been grouped under the classifications of railway tank cars and highway tank vehicles.

4.1.1.1 Railway tank cars. Railway tank cars used to transport 2-ethylhexanol are specifically regulated. A number of classifications are permitted; these are described in Table 2 (RTDCR 1974).

Figure 6 shows a typical railcar used to transport 2-ethylhexanol; Table 3 indicates railway tank car details associated with this drawing (TCM 1979; RTDCR 1974). Cars are equipped for unloading by pump or gravity through a bottom outlet provided with an inner plug valve. In addition to bottom unloading, the cars may be unloaded from the top by pump. In this case, the 2-ethylhexanol is withdrawn through an eduction pipe which extends from the bottom of the tank to the top operating platform where it terminates with an unloading connection valve. Air pressure is never used for unloading these tanks (BASF 1982).

4.1.1.2 Tank motor vehicles. 2-Ethylhexanol is also transported by aluminum or stainless steel tank motor vehicles. Highway tanks carrying 2-ethylhexanol are similar to the previously described railway tanks (BASF 1982).

The off-loading equipment and procedures for tank motor vehicles are similar to those for railway tank cars, to be discussed later. Tanks are usually unloaded from the top by pump.

4.2 Off-loading

4.2.1 Off-loading Equipment and Procedures for Railway Tank Cars. Prior to off-loading, certain precautions must be taken:

- The vented storage tank must be checked to make sure that it will hold the contents of the car.
- For night-time unloading, lights must have an explosion-proof rating.
- Personnel must not enter the car under any circumstances.
- Brakes must be set, wheels chocked, derails placed and caution signs displayed.
- A safe operating platform must be provided at the unloading point.
- Tools used during unloading must be spark-resistant.
- Tank car must be effectively grounded.

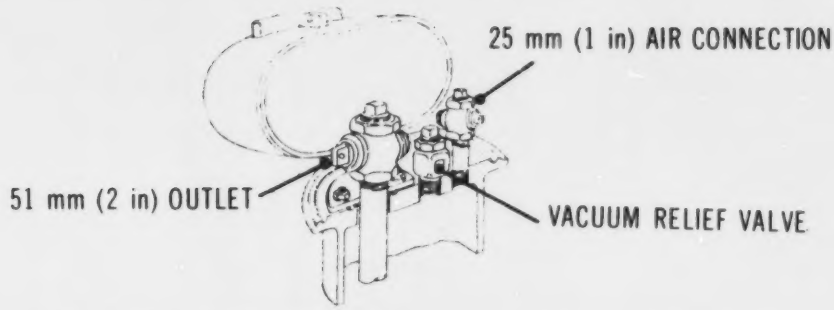
TABLE 2 RAILWAY TANK CAR SPECIFICATIONS

CTC/DOT Specification	Tank Material	Insulation	Test Pressure kPa (psi)	Dome	Bottom Outlet	Bottom Washout	Gauging Device
103W	steel	optional	414 (60)	required	optional	optional	optional
103ALW	aluminum alloy	optional	414 (60)	required	optional	optional	optional
104W	steel	optional	414 (60)	required	optional	optional	optional
105A100W	steel	required	690 (100)	none	prohibited	prohibited	standard
105A100ALW	aluminum alloy	required	690 (100)	none	prohibited	prohibited	standard
109A100ALW	aluminum alloy	optional	690 (100)	none	prohibited	optional	standard
111A60W1	steel	optional	414 (60)	none	optional	optional	required
111A60ALW1	aluminum alloy	optional	414 (60)	none	optional	optional	required
111A60F1	steel	optional	414 (60)	none	optional	optional	required
111A100W3	steel	required	690 (100)	none	optional	optional	required
111A100W4	steel	required	690 (100)	none	prohibited	prohibited	required
111A100W6	alloy steel	optional	690 (100)	none	optional	optional	required
112A200W	steel	none	1380 (200)	none	prohibited	prohibited	standard
112A400F	steel	none	2760 (400)	none	prohibited	prohibited	standard
114A340W	steel	none	2340 (340)	none	optional	optional	standard

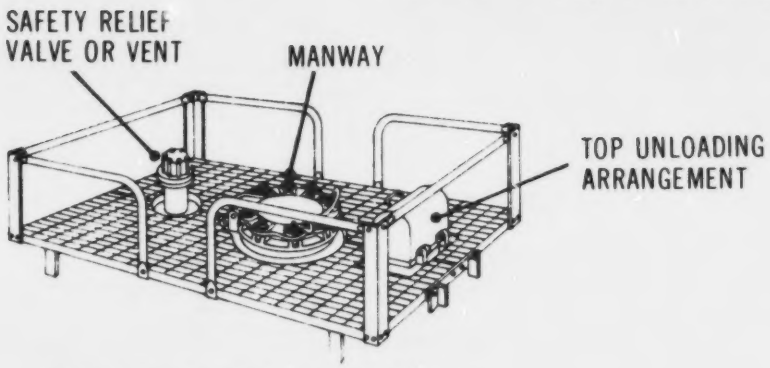
2–ETHYLHEXANOL

RAILWAY TANK CAR - CLASS 111A60W1

(Reference - TCM 1979; RTDCR 1974)



Detail of top unloading arrangement



Detail of loading platform

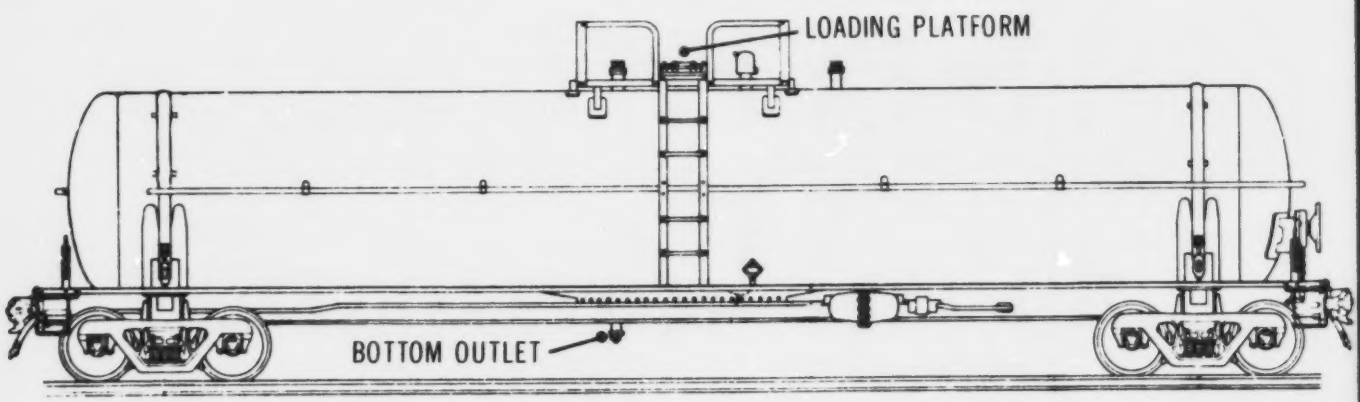


Illustration of tank car layout

TABLE 3 TYPICAL RAILWAY TANK CAR SPECIFICATIONS - CLASS 111A60W1 (TCM 1979; RTDCR 1974)

Description	Tank Car Size (Imp. Gal.)		
	16 700	17 200	20 000
Overall			
Nominal capacity	75 700 L (16 700 gal.)	78 000 L (17 200 gal.)	90 900 L (20 000 gal.)
Car weight- empty	33 900 kg (74 700 lb.)	33 900 kg (74 700 lb.)	38 900 kg (85 800 lb.)
Car weight- (max.)	119 000 kg (263 000 lb.)	83 500 kg (184 000 lb.)	119 000 kg (263 000 lb.)
Tank			
Material	Steel	Steel	Steel
Thickness	11.1 mm (7/16 in.)	11.1 mm (7/16 in.)	11.1 mm (7/16 in.)
Inside diameter	2.60 m (102 in.)	2.60 m (103 in.)	2.74 (108 in.)
Test pressure	414 kPa (60 psi)	414 kPa (60 psi)	414 kPa (60 psi)
Burst pressure	1640 kPa (240 psi)	1640 kPa (240 psi)	1640 kPa (240 psi)
Approximate Dimensions			
Coupled length	17 m (57 ft.)	17 m (57 ft.)	18 m (60 ft.)
Length over strikers	16 m (53 ft.)	16 m (53 ft.)	17 m (57 ft.)
Length of truck centres	13 m (42 ft.)	13 m (42 ft.)	14 m (45 ft.)
Height to top of grating	4 m (12 ft.)	4 m (12 ft.)	4 m (13 ft.)
Overall height	5 m (15 ft.)	5 m (15 ft.)	5 m (15 ft.)
Overall width (over grabs)	3.2 m (127 in.)	3.2 m (127 in.)	3.2 m (127 in.)
Length of grating	2-3 m (8-10 ft.)	2-3 m (8-10 ft.)	2-3 m (8-10 ft.)
Width of grating	1.5-2 m (5-6 ft.)	1.5-2 m (5-6 ft.)	1.5-2 m (5-6 ft.)
Loading/Unloading Fixtures			
Top Unloading			
Unloading connection	51 mm (2 in.)	51 mm (2 in.)	51 mm (2 in.)
Manway/fill hole	203-356 mm (8-14 in.)	203-356 mm (8-14 in.)	203-356 mm (8-14 in.)
Air connection	25-51 mm (1-2 in.)	25-51 mm (1-2 in.)	25-51 mm (1-2 in.)
Bottom Unloading			
Bottom outlet	102-152 mm (4-6 in.)	102-152 mm (4-6 in.)	102-152 mm (4-6 in.)
Safety Devices	Safety vent or valve		
Dome	None		
Insulation	Optional		

Two means of off-loading are used for rail cars, top off-loading and bottom off-loading (PC 1982). Proceed with top off-loading as follows:

- Relieve the tank of internal vapour pressure by cooling with water or venting at short intervals.
- After removing the protective housing from the discharge line at top of car, connect the 51 mm (2 in.) unloading line.
- Off-load the tanker by pumping.

Proceed with bottom off-loading in the following manner using gravity flow or pumping:

- Relieve internal pressure as previously mentioned.
- After connecting the unloading line to the 152 mm (6 in.) bottom outlet, open the inside bottom valve by turning the valve rod handle at the top of the car.
- Off-load the car by gravity or pump.

4.2.2 Specifications and Materials for Off-loading Equipment. The materials of construction for off-loading system components discussed in this Section along with specifications refer to those generally used. It is recognized that other materials may be used for particular applications, as indicated in Table 4. The components of a typical off-loading system that will be discussed include pipes and fittings, flexible connections, valves, gaskets and pumps.

Schedule 40 seamless ASTM A106 carbon steel pipes and fittings are recommended. Flanged joints should be used and these should be welded, because threaded pipes and fittings tend to leak after a very short time. Stress relief at the weld will also lengthen the serviceability of the pipe. The pipeline should be tested with air at pressures from 345 to 518 kPa (50 to 75 psi) and all leaks carefully stopped. If leaks develop in service, the only satisfactory way to repair them is to chip out the bad weld and reweld, or to replace the section of pipe.

The unloading line should be 51 mm (2 in.) pipe because this is the standard fitting on 2-ethylhexanol tank cars; however, process pipe may be almost any size. Pipe under 25 mm (1 in.), however, is not recommended. Outdoor lines must be self-draining.

Some installations of flexible line are made with standard fittings using a number of screwed elbows. For valving, cast iron or cast steel diaphragm valves will serve adequately. Viton may be used as a gasket material at normal temperature ranges.

A centrifugal pump with "wet end" material or 316 stainless steel gives good results. There are no special requirements (BASF 1982).

4.3 Compatibility with Materials of Construction

The compatibility of 2-ethylhexanol with materials of construction is indicated in Table 4. The unbracketed abbreviations are described in Table 5. The rating system for this report is briefly described below.

Recommended: This material will perform satisfactorily in the given application.

Conditional: Material will show deterioration in the given application; however, it may be suitable for intermittent or short-term service.

Not Recommended: Material will be severely affected in this application and should not be used.

TABLE 4 COMPATIBILITY WITH MATERIALS OF CONSTRUCTION

	Material of Construction		
Application	Recommended	Conditional	Not Recommended
1. Pipes and Fittings	CS CS with glass-lining CR hoses NR hoses (BASF 1982)	CR NBR, NR (CCPA 1983)	
2. Valves	Cast steel, Cast steel glass-lined		
3. Pumps	All iron Cast steel Cast steel, glass-lined (BASF 1982)		
4. Storage	CS Aluminum SS (BASF 1982)		
5. Others			NBR CSM (GPP)

TABLE 5 MATERIALS OF CONSTRUCTION

Abbreviation	Material of Construction
	Aluminum
CR	Polychloroprene (Neoprene)
CS	Carbon Steel
CSM	Chlorosulphonated Polyethylene (Hypalon)
	Fluorine Rubber (Viton)
	Glass
	Iron
NBR	Acrylonitrile/Butadiene Rubber (Nitrile, Buna N)
NR	Natural Rubber
	Nickel-Copper Alloy (Monel)
SS	Stainless Steel

5 CONTAMINANT TRANSPORT

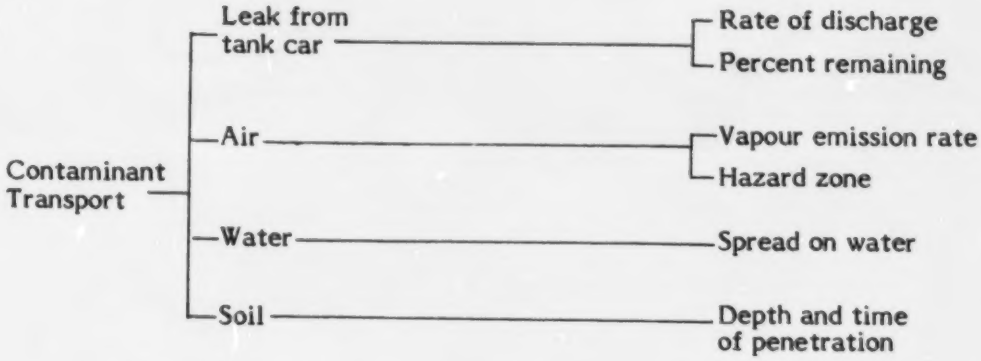
5.1 General Summary

2-Ethylhexanol is a colourless, oily liquid. When spilled, it will form a liquid pool, spreading on the surface of a water body or on the ground, being adsorbed onto the soil.

When spilled on water, the slick has a natural tendency to spread. Since it is only slightly soluble and less dense than water, only a very small amount will be dissolved in the water.

2-Ethylhexanol when spilled on the ground is gradually adsorbed onto the soil, at a rate dependent on the soil type and its degree of saturation with water. At the same time, the downward transport of the liquid toward the groundwater table may cause environmental problems.

The following factors are considered for the transport of a 2-ethylhexanol spill in the air, water and soil media:



It is important to note that, because of the approximate nature of the contaminant transport calculations, the approach adopted throughout has been to use conservative estimates of critical parameters so that predictions are approaching worst case scenarios for each medium. This may require that the assumptions made for each medium be quite different and to some extent inconsistent. As well as producing worst case scenarios, this approach allows comparison of the behaviours of different chemicals under consistent assumptions.

5.2 Leak Nomograms

5.2.1 Introduction. 2-Ethylhexanol is commonly transported in railway tank cars as a nonpressurized liquid. While the capacities of the tank cars vary widely, one tank car

size has been chosen throughout the EnviroTIPS series for development of the leak nomograms. It is approximately 2.75 m in diameter and 13.4 m long, with a carrying capacity of about 80 000 L.

If a tank car loaded with 2-ethylhexanol is punctured on the bottom, all of the contents will drain out by gravity. The aim of the nomograms is to provide a simple means to obtain the time history of the conditions in the tank car and the venting rate of the liquid. Because of the relatively low volatility of 2-ethylhexanol and the fact that the tank cars are not pressurized, no leak nomograms have been prepared for vapour release from a puncture in the top of the tank.

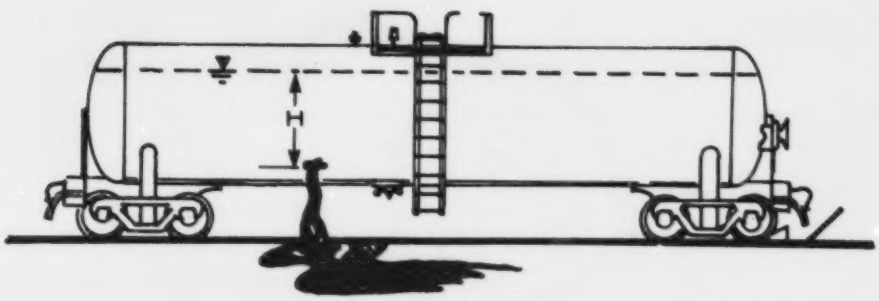


FIGURE 7 TANK CAR WITH PUNCTURE HOLE IN BOTTOM

The rate of outflow (q) from a vent hole in the bottom of the tank car is defined by the standard orifice equation (Streeter 1971). The venting rate (q) is a function of hole size (A) and shape, the height of the fluid above the puncture hole (H), and a coefficient of discharge (Cd).

As the gravitational force predominates over viscous and other forces for a wide range of fluid conditions, the rate of discharge is relatively independent of fluid temperature and viscosity (Rouse 1961). Consequently, it is reasonable to assume a constant discharge coefficient for 2-ethylhexanol for a wide range of temperature and viscosity. This can be equally well applied to a wide range of chemicals having significant variation in viscosity. For the purposes of nomogram preparation, a constant discharge coefficient of 0.8 has been assumed.

5.2.2 Nomograms.

5.2.2.1 Figure 8: Percent remaining versus time. Figure 8 provides a means of estimating the percent of liquid remaining in the standard tank car after the time of puncture, for a number of different hole diameters. The hole diameter is actually an equivalent diameter and can be applied to a noncircular puncture.

The standard tank car is assumed to be initially full (at t = 0) with a volume of about 80 000 L of 2-ethylhexanol. The amount remaining at any time (t) is not only a function of the discharge rate over time, but also of the size and shape of the tank car.

5.2.2.2 Figure 9: Discharge rate versus time. Figure 9 provides a means of estimating the instantaneous discharge rate (L/s) at any time (t) after the time of puncture, for a number of equivalent hole diameters. The nomogram is only applicable to the standard tank car size with an initial volume of 80 000 L.

5.2.3 Sample Calculations.

i) Problem A

The standard tank car filled with 2-ethylhexanol has been punctured on the bottom. The equivalent diameter of the hole is 150 mm. What percent of the initial 80 000 L remains after 10 minutes?

Solution to Problem A

- Use Figure 8
- With t = 10 min and d = 150 mm, the amount remaining is about 36 percent or 28 800 L

ii) Problem B

With the same conditions as Problem A, what is the instantaneous discharge rate from the tank 10 minutes after the accident?

Solution to Problem B

- Use Figure 9
- With t = 10 min and d = 150 mm, the instantaneous discharge rate (q) = 70 L/s

5.3 Dispersion in the Air

Because no TLV® for 2-ethylhexanol has been established and due to its low volatility, this chemical is not modelled with respect to its potential dispersion in air.

FIGURE 8

2–ETHYLHEXANOL

PERCENT REMAINING VS TIME

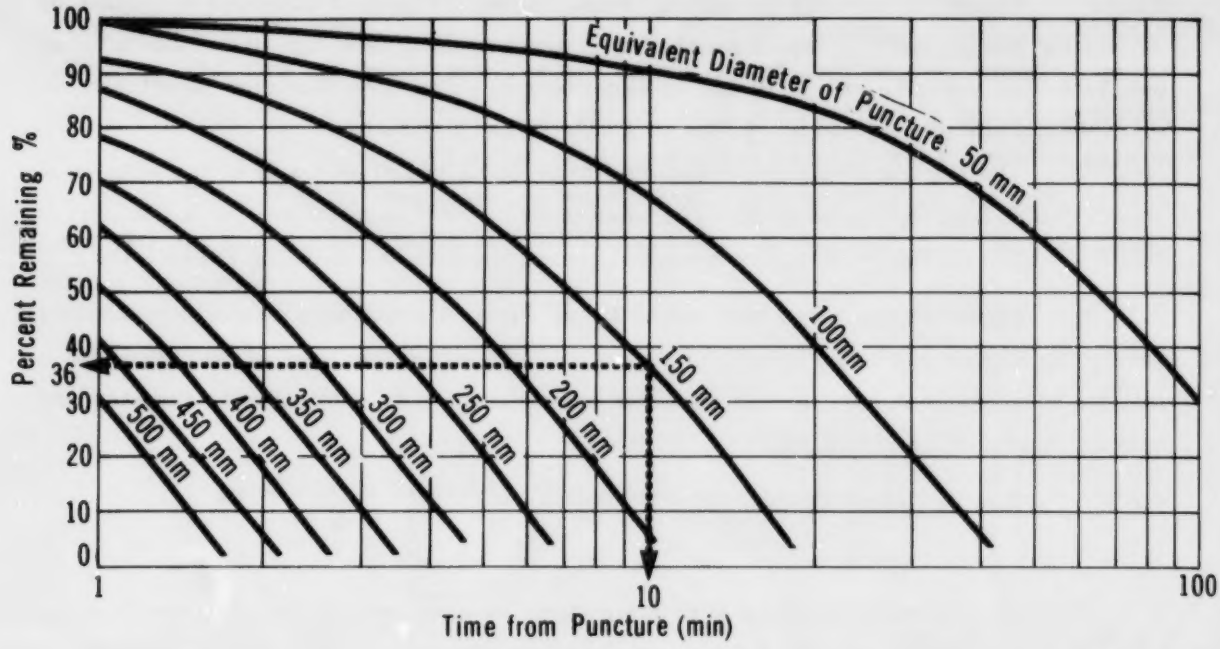
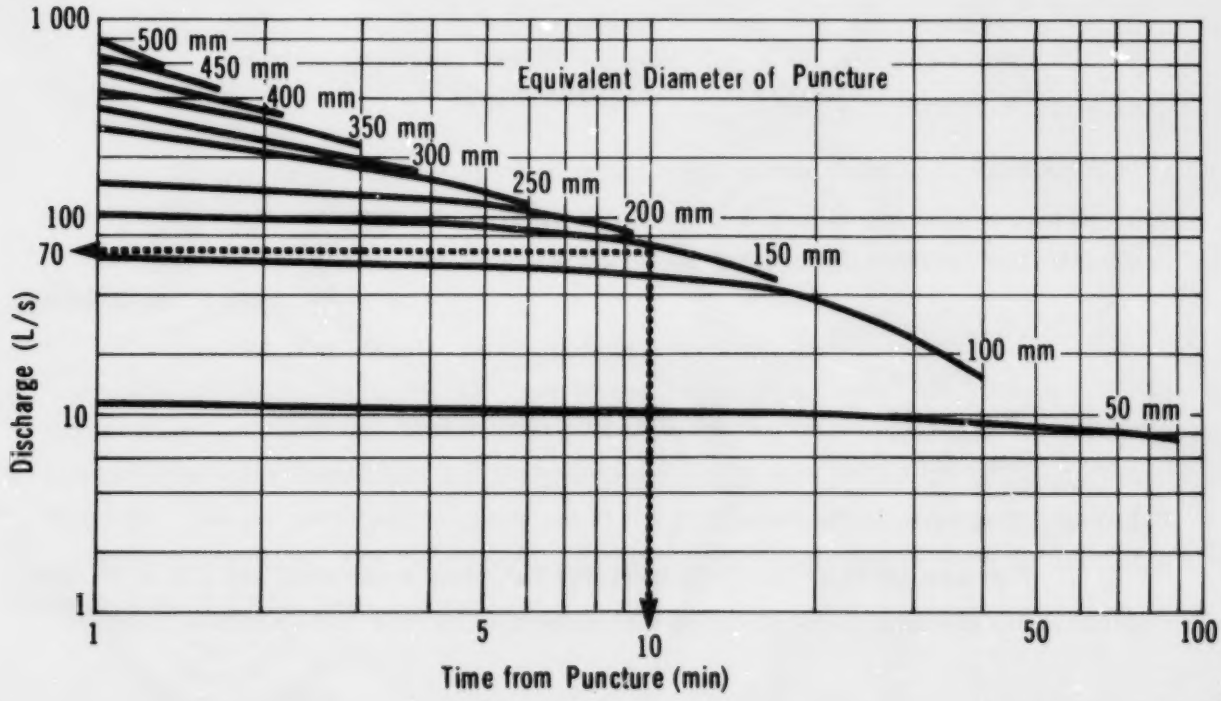


FIGURE 9

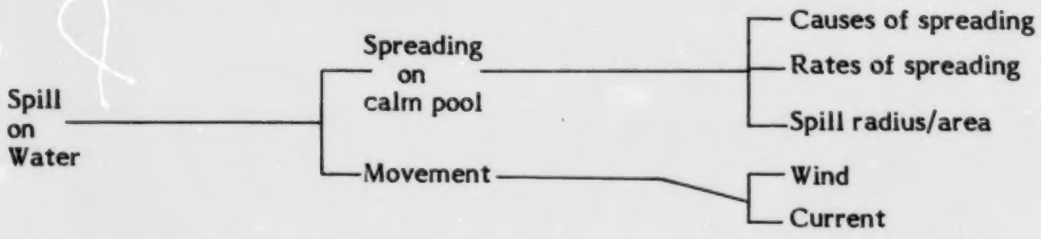
2–ETHYLHEXANOL

DISCHARGE RATE VS TIME



5.4 Behaviour in Water

5.4.1 Introduction. The rate of spreading on water is based on the balance between forces tending to spread the liquid (gravity and surface tension) and those tending to resist spreading (inertial and viscous forces).



5.4.2 Nomograms. The following nomograms are presented to simplify calculations:

Figure 10: spill radius versus time (still water - unconfined) for various sizes of spills; maximum spill radius indicated

Figure 11: length of channel affected versus equivalent spill radius (still water - confined) for a number of stream widths

Figure 12: translation distance versus time for a range of surface water velocities

Figure 13: vectoral addition of surface current and wind

5.4.2.1 Figure 10: Spill radius versus time (still water - unconfined). Figure 10 provides a means of calculating the radius/area of an unconfined slick of 2-ethylhexanol for a known mass of spill and at a defined time from the occurrence of the spill. The equations representing the spreading of the spill on water are presented in the Introduction Manual. A critique of the spreading model (Eisenberg 1975) suggests that the equations are valid for cases where the viscosity of the spilled liquid is greater than or equal to 0.2 times the viscosity of water ($U_L \geq 0.2\ U_W$).

For the purposes of the nomogram presented, the water/spill temperature has been taken at 20°C, representing a reasonable maximum for surface water bodies. This condition maximizes the spill size at any time of interest. If the indicated pool radius is larger than the theoretical maximum radius, use the theoretical maximum pool radius.

5.4.2.2 Figure 11: Length of channel affected versus equivalent spill radius (still water - confined). If the distance between the banks of the water body is less than the spill diameter, the slick will be confined. Using the effective radius of spill from Figure 10, the approximate length of channel affected by the spill can be computed from Figure 11, if the stream width is known.

FIGURE 10

2-ETHYLHEXANOL

SPILL RADIUS VS TIME
(still water - unconfined)

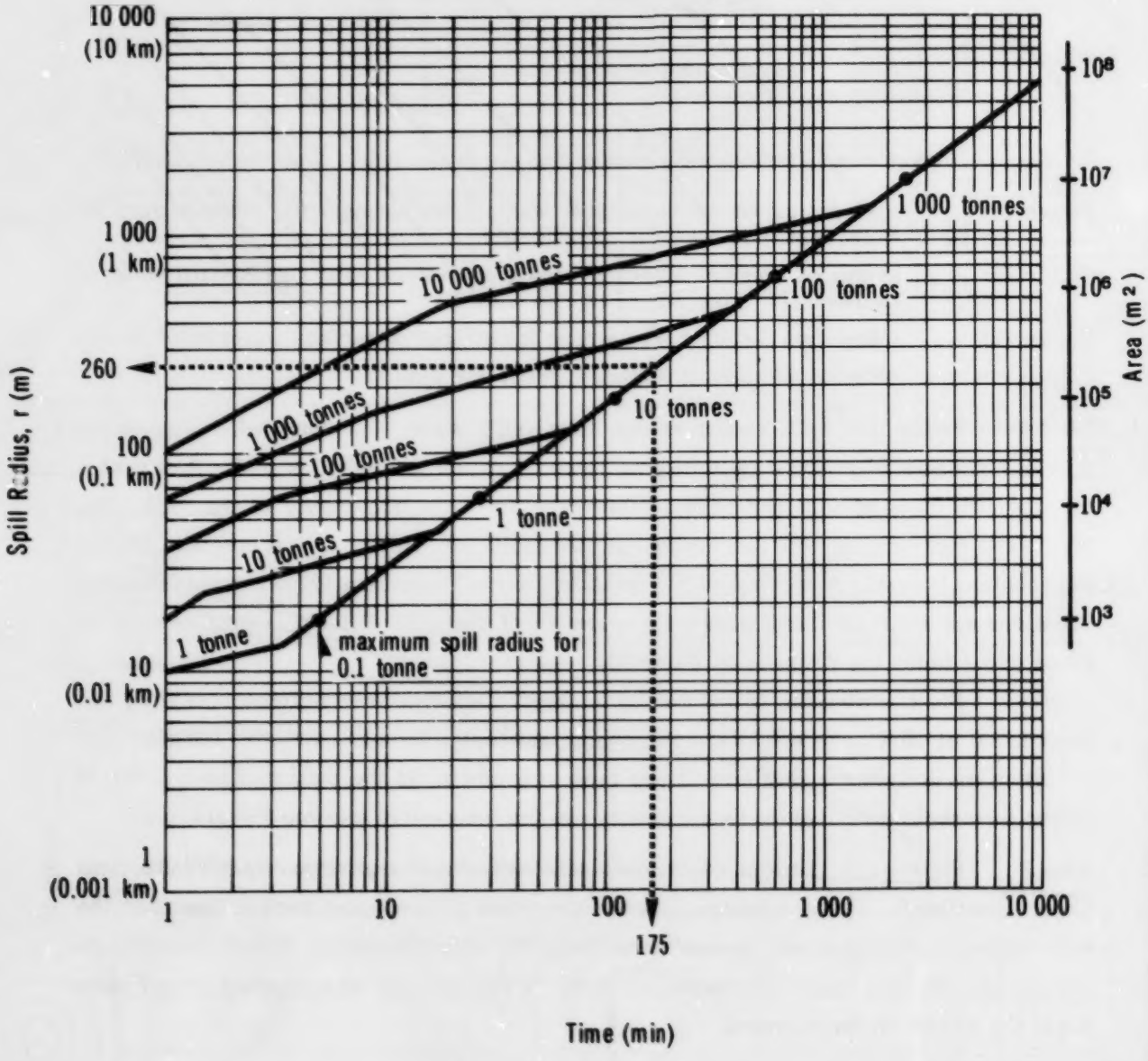
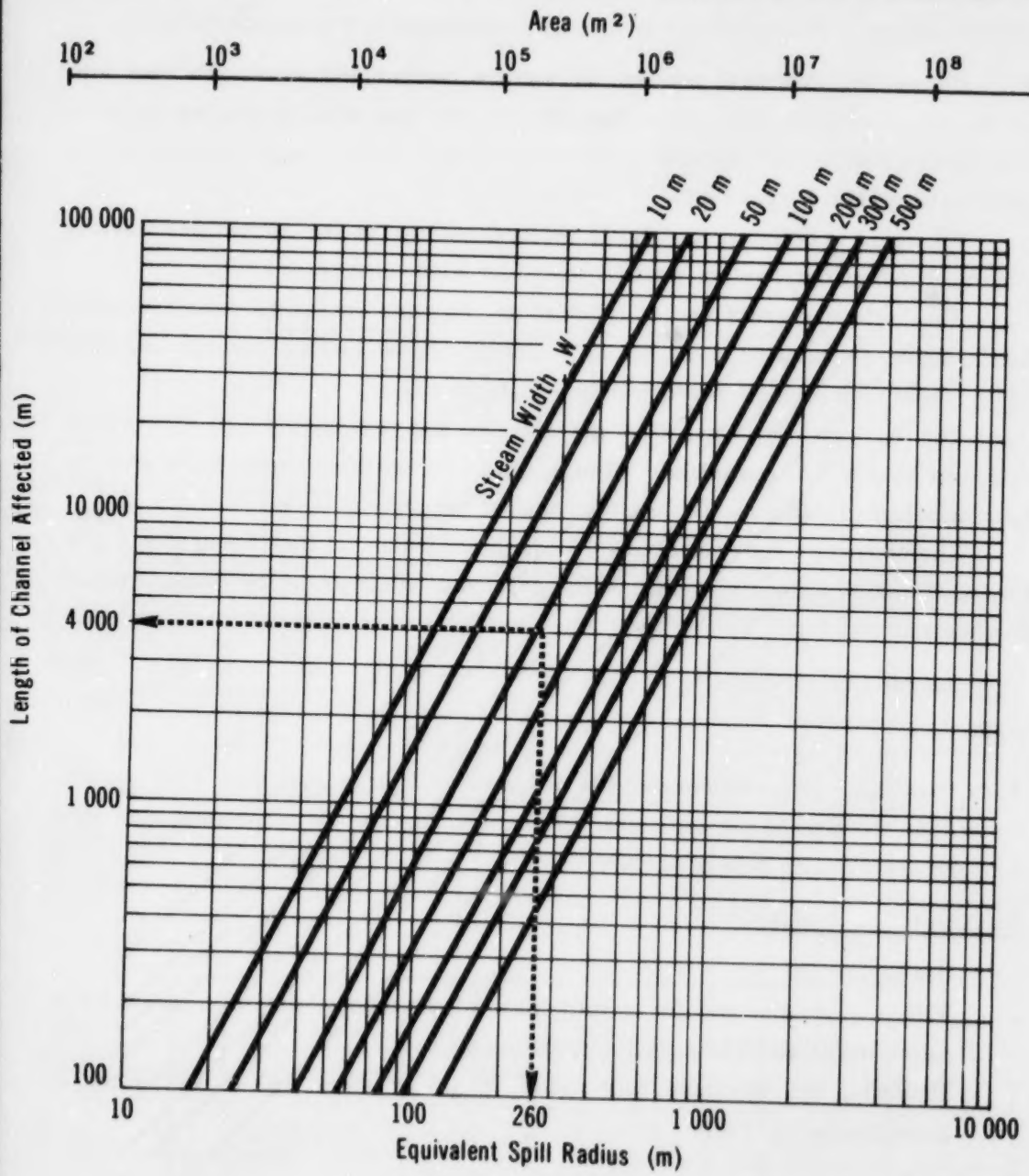


FIGURE 11

2–ETHYLHEXANOL

LENGTH OF CHANNEL AFFECTED VS SPILL RADIUS (still water - confined)



5.4.2.3 Figure 12: Translation distance versus time (no wind). Figure 12 presents a simple relationship between velocity, time and distance. The distance a spill will be translated in time by a flowing stream is directly proportional to the surface current.

5.4.2.4 Figure 13: Vectoral addition of surface current and wind. To take into account the effect of both wind and surface current, the spill slick is assumed to move with a velocity given by the vectoral addition of current velocity and 3 percent of the wind velocity (Raj 1974; Fingas 1980).

Figure 13 is designed to simplify vectoral addition of the current and velocity components. The horizontal velocity axis is scaled for wind velocity, in km/h.

The surface current vector is added to the wind vector by determining its direction relative to the wind direction. The length of the surface current vector is defined by the vertical surface current velocity scale, in m/s.

The resultant vector describes the direction and velocity the spill slick will be moving due to wind and current effects. The length of the resultant vector represents the spill translation velocity (m/s) when measured against the vertical scale.

The nomogram does not account for deformation of the slick shape when influenced by wind and/or surface currents, or for any losses which occur by evaporation or any other means.

5.4.3 Sample Calculations.

i) Problem A

A 20 tonne spill of 2-ethylhexanol has occurred on a large lake. The wind is calm. Determine the size of the spill after 20 minutes, together with the maximum spill size and approximate time of occurrence.

Solution to Problem A

- Use Figure 10
- With t = 20 min and for a spill mass of 20 tonnes, the spill radius (r) is estimated at about 60 m by interpolation
- Similarly, the maximum spill radius (r_{max}) of about 260 m will occur in approximately 175 min

ii) Problem B

The slick in Problem A is confined to a calm channel, approximately 50 m in width. What is the maximum length of channel affected by this spill?

FIGURE 12

2-ETHYLHEXANOL

TRANSLATION DISTANCE vs TIME (No wind)

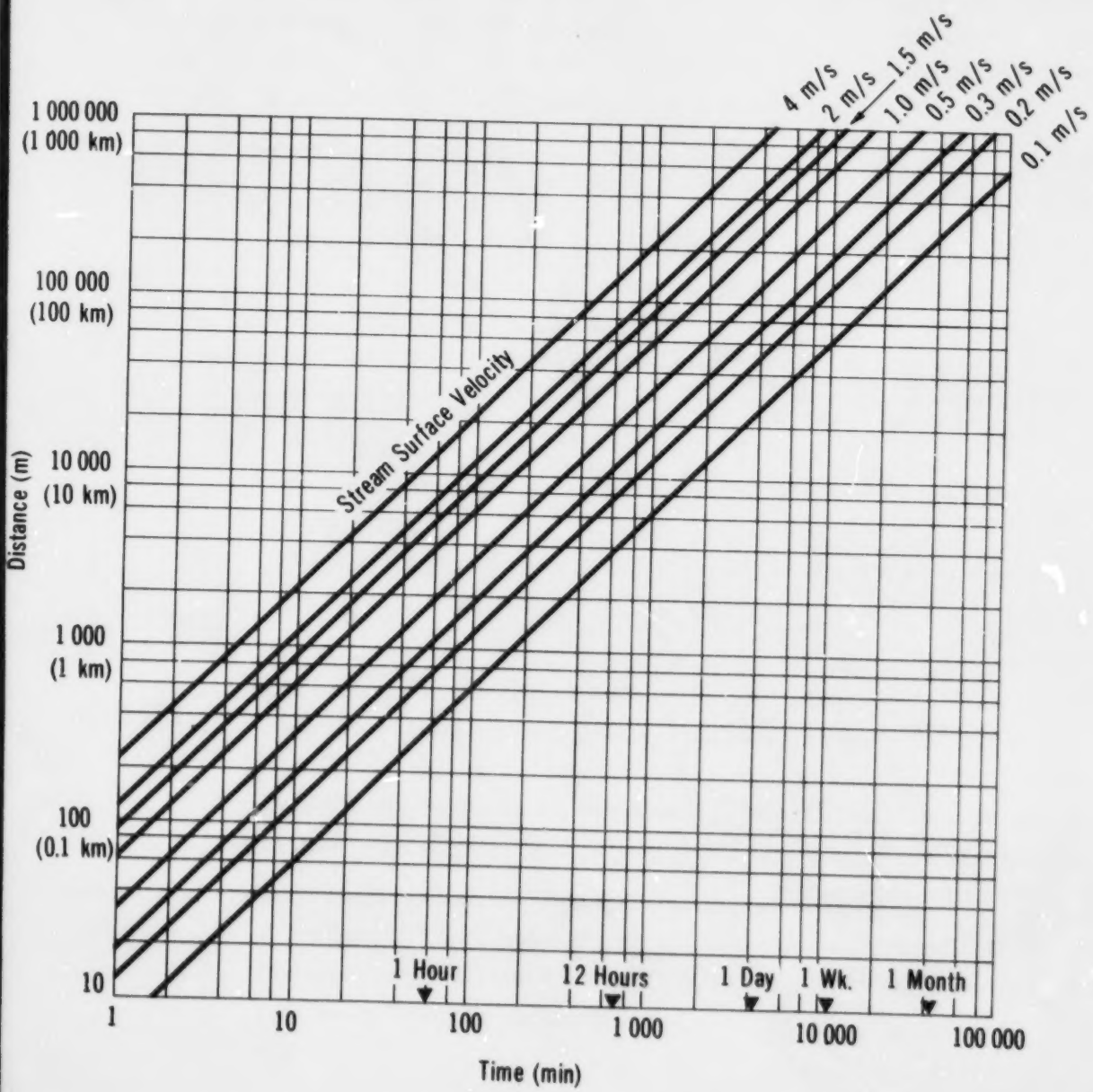
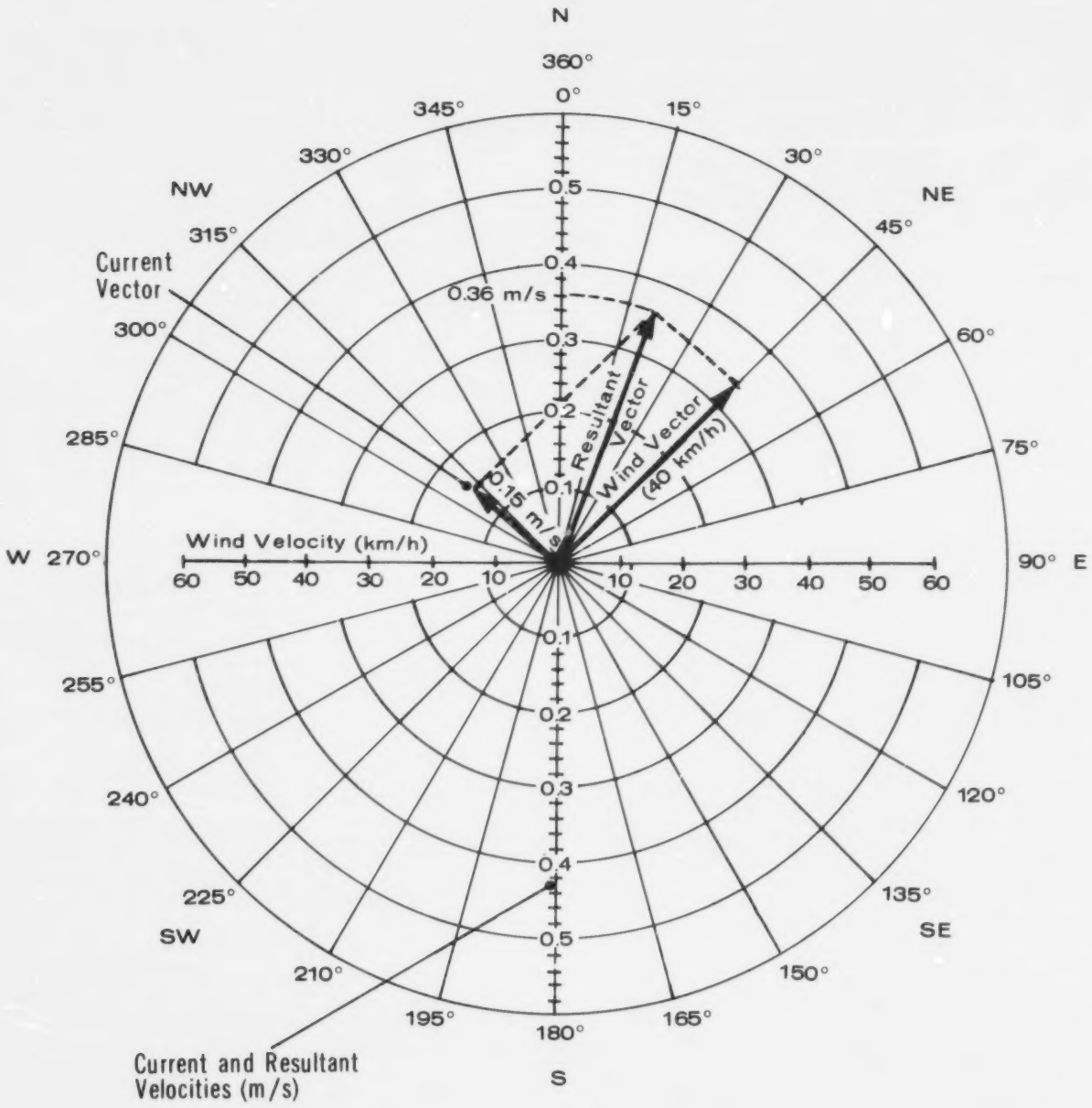


FIGURE 13

2-ETHYLHEXANOL

VECTORAL ADDITION OF SURFACE CURRENT AND WIND



Solution to Problem B

- Figure 10 (or Solution to Problem A) gives r_{max} = 260 m for a 20 tonne spill
- Use Figure 11: with r_{max} = 260 m and a stream width of 50 m, the maximum length of channel affected under still conditions is about 4000 m (4 km)

iii) Problem C

The 20 tonne spill in Problem A is being affected by a wind velocity of 40 km/h from the southwest and a surface current of 0.15 m/s at 90° from the wind direction (i.e., flow is northwest). What is the resultant direction and speed of the slick and the distance the slick has moved when it reaches its maximum size?

Solution to Problem C

Step 1: Define wind vector

- Use Figure 13
- Determine length of wind vector for 40 km/h against horizontal wind velocity scale
- Draw wind vector at appropriate length and in northeasterly direction starting at origin

Step 2: Define surface current vector

- Determine length of surface current vector of 0.15 m/s against vertical axis on Figure 13
- Draw surface current vector at appropriate length and in northwesterly direction, starting from head of wind vector

Step 3: Define resultant vector

- Draw resultant vector from origin to head of current vector
- Direction of translation as given by resultant vector is about 20° east of north
- Define translation velocity by measuring length of the resultant vector against vertical scale. Spill translation velocity is estimated at 0.36 m/s

Step 4: Determine distance travelled when spill reaches maximum radius

- From Figure 10 (or Problem A), r_{max} = 260 m at t = 175 min (10 500 s)
- Distance travelled = 10 500 s x 0.36 m/s = 3800 m, by the time the spill reaches its maximum radius

5.5 Subsurface Behaviour: Penetration into Soil

5.5.1 Introduction. The general principles of contaminant transport in soil and their application to this work are described in the Introduction Manual. Specific items related to and the development of nomograms for it are presented below.

2-Ethylhexanol is relatively insoluble in water. Consequently, when spilled onto soil, its infiltration and transport downward through the soil involve multi-phase phenomena. The phases of concern are liquid 2-ethylhexanol, water, soil, and gas or vapours.

Unfortunately, sufficient data do not exist to permit a detailed assessment of contaminant transport in a specific circumstance. A few extensive field investigations have been carried out, especially involving spills of oil, gasoline and PCBs. However, very limited information exists for 2-ethylhexanol. Consequently, it is necessary to simplify the soil and groundwater conditions and to express contaminant behaviour through analogy to other more extensively studied materials. A pattern for the downward movement of immiscible fluids such as 2-ethylhexanol in soil has been prepared by comparison to oil spilled onto soil surfaces (Blokker 1971; Freeze and Cherry 1979).

It is assumed that when the spill occurs, the soil contains water only up to its field capacity and that this condition prevails down to the groundwater table. The spilled liquid fills the pores at the soil surface and begins to penetrate downward. It is assumed that 2-ethylhexanol moves downward through the soil as a saturated slug, but leaving behind a constant residual amount (S_o) within the soil pores.

Downward transport will continue until the volume of 2-ethylhexanol spilled per unit area (B_o) equals the amount retained in the soil as S_o. Some lateral spreading may occur due to capillary action. If B_o is greater than the volume that can be retained as S_o above the groundwater table, the excess liquid will spread as a pancake within the saturated groundwater capillary fringe. The resultant contaminated zone consisting of a "vertical" column and "horizontal" pancakes of soil containing the residual amount of 2-ethylhexanol, S_o, is shown schematically in Figure 14.

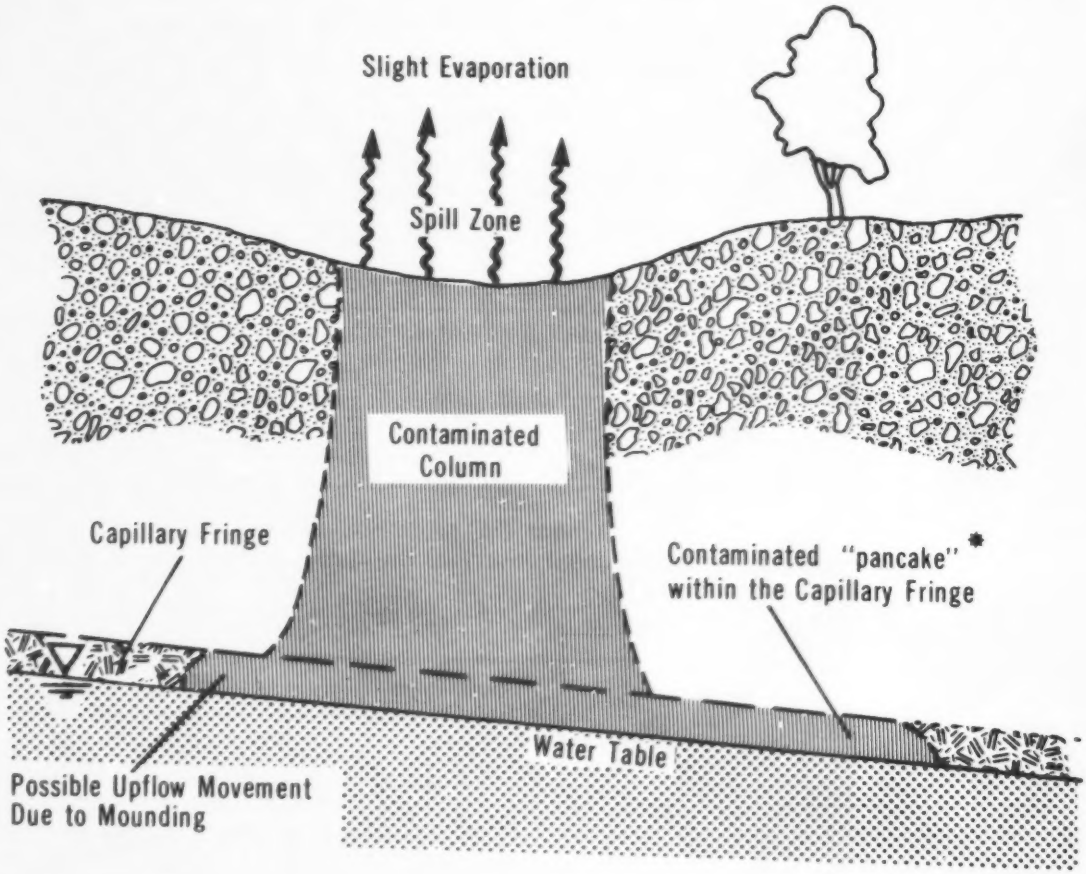
5.5.2 Equations Describing 2-Ethylhexanol Movement into Soil. The equations and assumptions used to describe contaminant movement downward through the unsaturated soil zone toward the groundwater table have been described in the Introduction Manual. Transport velocities have been based on Darcy's Law assuming saturated piston flow.

5.5.3 Saturated Hydraulic Conductivity of 2-Ethylhexanol in Soil. The saturated hydraulic conductivity (K_o), in m/s, is given by:

FIGURE 14

2–ETHYLHEXANOL

SCHEMATIC SOIL TRANSPORT



Soil: Coarse Sand

–Porosity (n) = 0.35

–intrinsic Permeability (k) = 10^{-9} m^2

–Field Capacity (θ_{fc}) = 0.075

*Column and Pancake Contain Residual $S_o = 0.05$

$$K_o = \frac{(\rho g)k}{\mu}$$

where:

- k = intrinsic permeability of the soil (m^2)
- ρ = mass density of the fluid (kg/m^3)
- μ = absolute viscosity of the fluid (Pa·s)
- g = acceleration due to gravity = 9.81 m/s^2

The appropriate properties of 2-ethylhexanol are given in the following chart:

Property	2-Ethylhexanol, 20°C
Mass density (ρ), kg/m^3	834
Absolute viscosity (μ), Pa·s	9.8×10^{-3}
Saturated hydraulic conductivity (Ko), m/s	$(1.63 \times 10^7)k$

5.5.4 Soils. The Introduction Manual describes the three soils selected for this work. Their relevant properties are:

	Soil Type		
Property	Coarse Sand	Silty Sand	Clay Till
Porosity, n (m^3/m^3)	0.35	0.45	0.55
Intrinsic permeability, k (m^2)	10^{-9}	10^{-12}	10^{-15}
Field capacity, θ_{fc} (m^3/m^3)	0.075	0.3	0.45
Residual fraction, S_o (m^3/m^3)	0.05	0.1	0.2

5.5.5 Penetration Nomogram. Nomograms for the penetration of 2-ethylhexanol into the unsaturated zone above the groundwater table were prepared for each soil.

The nomograms show the total depth of penetration (B) versus penetration time (t_p) for various volumes spilled per unit area of soil (B_o). Temperatures of 4°C and 20°C were used. Calculations were based on the equations developed in the Introduction Manual.

$$v = -K_o \frac{(dh)}{(dl)} \qquad t_p = \frac{B}{v}$$

$$\frac{dh}{dl} = -1 \qquad B = \frac{B_o}{n_{so}}$$

A flowchart for use of the nomograms is shown in Figure 15. The nomograms are presented in Figures 16, 17 and 18.

5.5.6 Sample Calculation. A 20 tonne spill of 2-ethylhexanol has occurred on coarse sandy soil. The temperature is 20°C; the spill radius is approximately 8.6 m. Calculate the depth and time of penetration.

Solution

Step 1: Define parameters

- Mass spilled = 20 000 kg (20 tonnes)
- T = 20°C
- Mass density = 834 kg/m^3
- r = 8.6 m

Step 2: Calculate volume and area of spill

- $V = \frac{M}{e} = \frac{2 \times 10^4 \text{ kg}}{834 \text{ kg/m}^3} = 24 \text{ m}^3$
- $A = r^2 = 232 \text{ m}^2$

Step 3: Calculate volumetric loading, B_o

- $B_o = \frac{V}{A} = \frac{24}{232} = 0.1 \text{ m}^3/\text{m}^2$

Step 4: Estimate depth of penetration (B) and time of penetration (t_p)

- For coarse sand, $B_o = 0.1 \text{ m}^3/\text{m}^2$
- B = 5.9 m, t_p = 5.8 min

FIGURE 15

2-ETHYLHEXANOL

FLOWCHART FOR NOMOGRAM USE

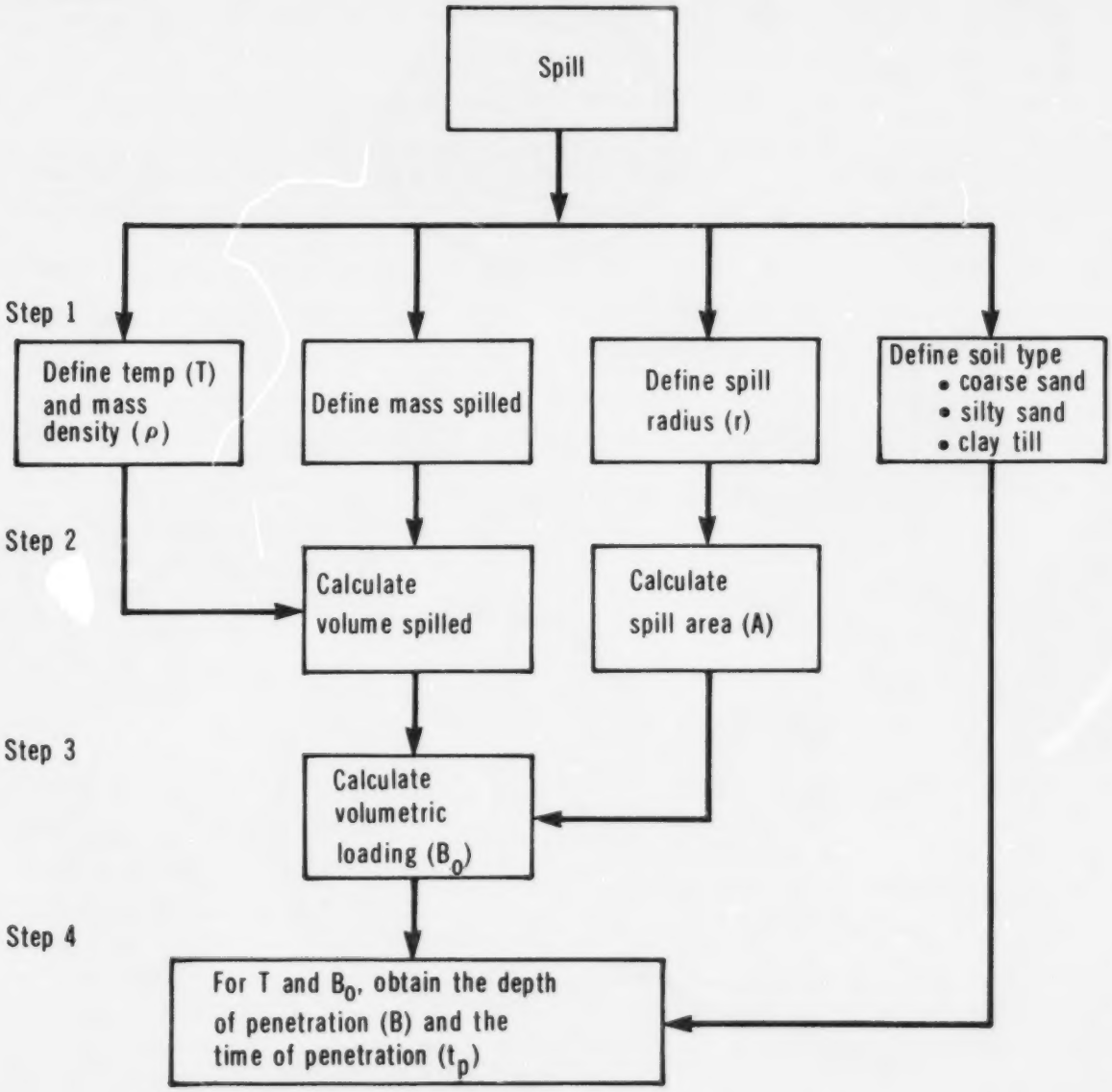


FIGURE 16

2-ETHYLHEXANOL

PENETRATION IN COARSE SAND

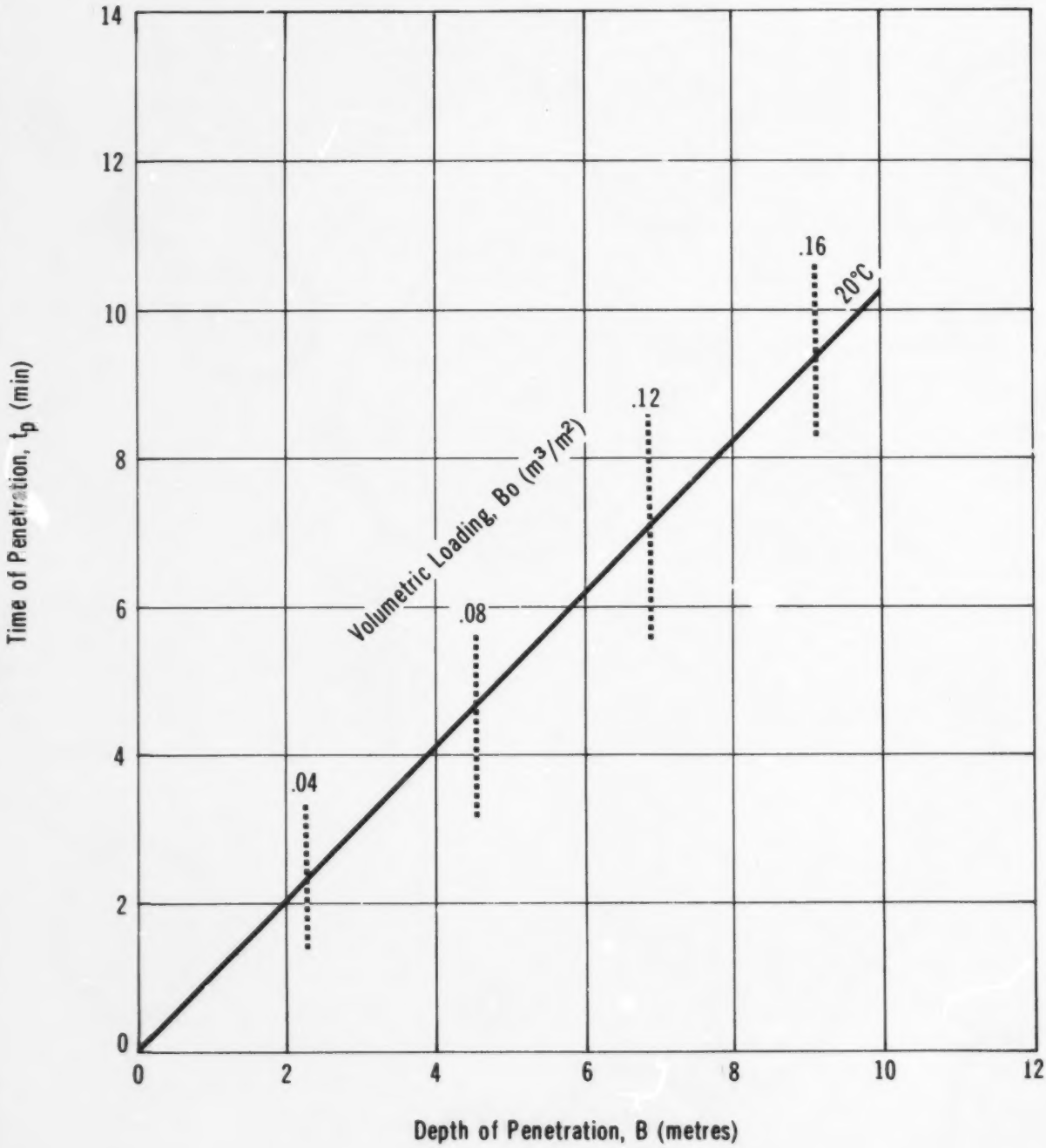


FIGURE 17

2-ETHYLHEXANOL

PENETRATION IN SILTY SAND

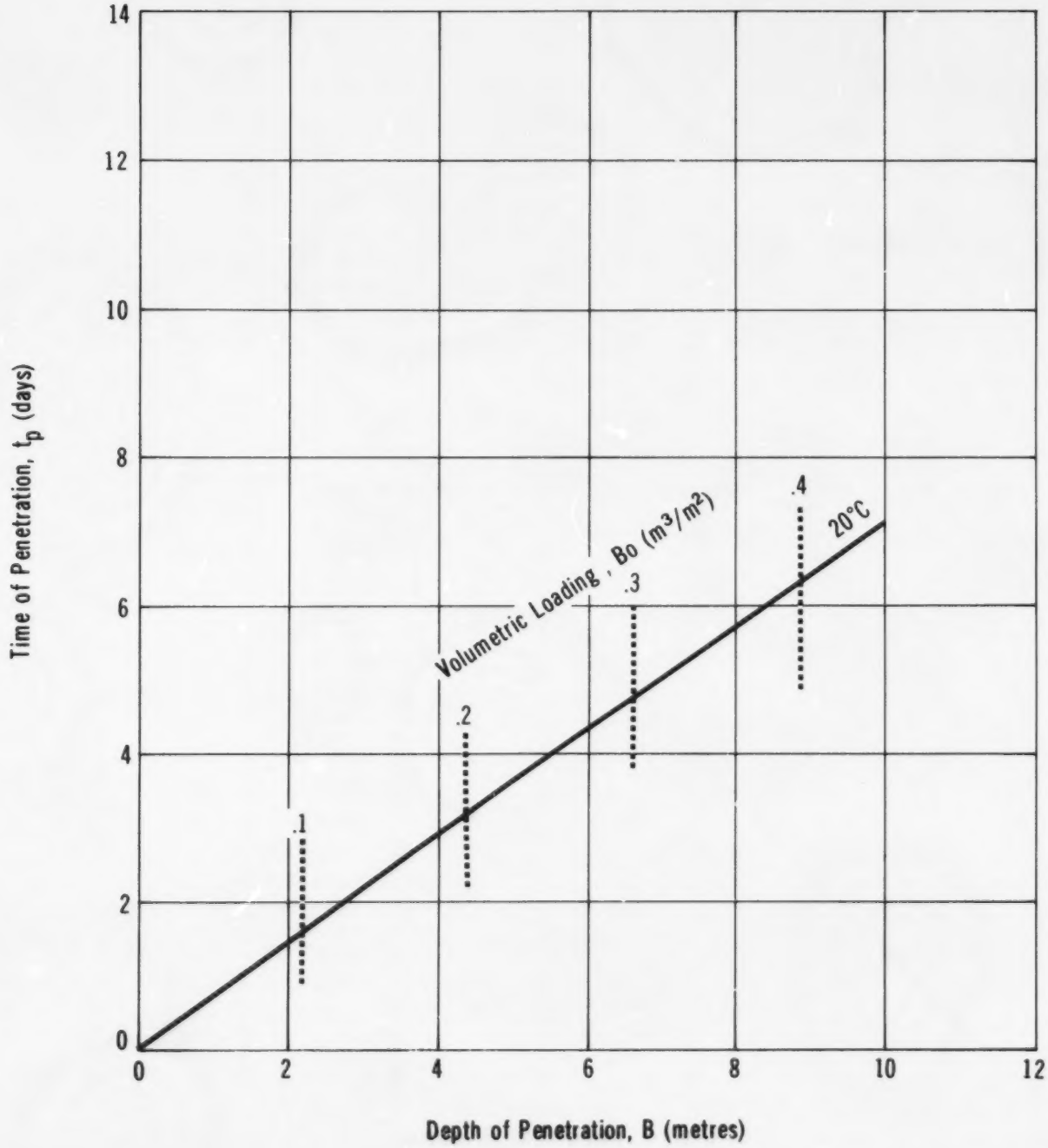
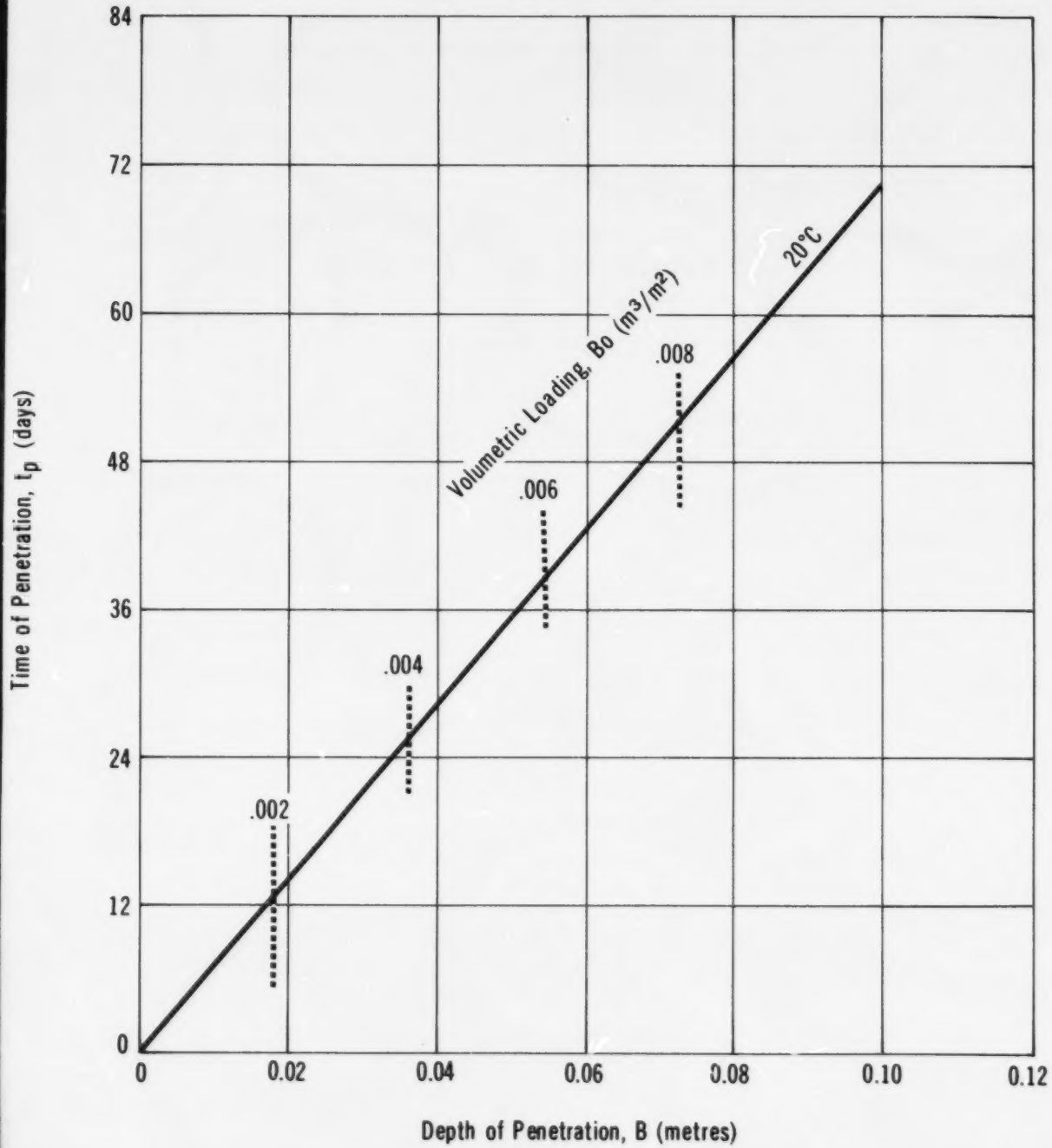


FIGURE 18

2–ETHYLHEXANOL

PENETRATION IN CLAY TILL



6 ENVIRONMENTAL DATA

6.1 Suggested or Regulated Limits

6.1.1 Water. No specific limits have been recommended in Canada or the United States.

6.1.2 Air. No specific limits have been recommended in Canada or the United States.

6.2 Aquatic Toxicity

6.2.1 U.S. Toxicity Rating. No toxicity rating has been assigned.

6.2.2 Measured Toxicities.

Conc. (mg/L)	Time (hours)	Species	Result	Water Conditions	Reference
Fish Toxicity Tests					
10 to 100	48	Golden Ides	LC_{50}		BASF PSDS 1981
<75	120	Goldfish	LC_{50}	static, 20°C, pH 7.0, HD 180	JWPCF 1980
32 to 37	96	Rainbow trout	LC_{50}	static, 15°C, pH 8.5, HD 43	JWPCF 1979; Dave 1978
5	24	Sea lamprey	no effect	12°C, Lake Huron	PB 216658
Invertebrates					
19	24	Brine shrimp	TL_m	Saltwater	CHRIS 1978
34	48	Midge larvae	LC_{50}	-	Streufort 1980

6.2.3 Aquatic Studies. 2-Ethylhexanol may harm vegetation and fish (BASF PSDS 1981).

6.3 Degradation

B.O.D. % Theor.	Days	Method	Reference
88%	5	BOD	CHRIS 1978
50 to 100%	5	(BOD_5:COD) x 100	BASF PSDS 1981

There is no inhibition of bacteria in effluent if the material is properly introduced into acclimated biological treatment facility (BASF PSDS 1981).

6.4 Long-term Fate and Effects

There is no food chain concentration potential (CHRIS 1978).

7 HUMAN HEALTH

There is a limited amount of information in the published literature concerning the toxicological effects of test animal and human exposures to 2-ethylhexanol. Much of the published information pertaining to the health effects of this chemical deals with its irritant effects on the eyes and skin, and the consequences of ingestion. There was no information encountered in the literature on the effects of 2-ethylhexanol on reproduction, nor its mutagenicity or carcinogenicity. Little information is available on the effects of chronic exposure to this chemical.

2-Ethylhexanol has been reported in the EPA TSCA inventory. The data summarized here are representative of information in the literature.

7.1 Recommended Exposure Limits

The exposure standards for 2-ethylhexanol are based upon its irritant properties.

Guideline (Time)	Origin	Recommended Level	Reference
Time-weighted Averages (TWA)			
	USSR	9 ppm (50 mg/m^3)	GE 1979; Verschueren 1977
MAC (Average)	Czech.	200 mg/m^3	ILO 1980
MAK-D (8 h 45 min) (maximum acceptable concentration)	GDR	400 mg/m^3	ILO 1980
Short-term Exposure Limits (STEL)			
MAC (Maximum)	Czech.	400 mg/m3	ILO 1980

7.2 Irritation/Contact Data

7.2.1 Skin Contact.

Exposure Level (and Duration)	Effects	Reference
SPECIES: Human		
-	Moderately irritating to skin	TDB (on-line) 1981

Exposure Level (and Duration)	Effects	Reference
SPECIES: Rabbit		
> 2600	LD_{50}	Scala 1973
2600 mg/kg (24 h)	Moderate irritation	RTECS 1979; Patty 1982
2000 mg/kg	LD_{50}	Patty 1982
2380 mg/kg	LD_{50}	GE 1979
415 mg, open skin test	Mild irritation	TDB (on-line) 1981
SPECIES: Guinea Pig		
> 8300 mg/kg	LD_{50}	Patty 1982

7.2.2 Eye Contact.

Exposure Level (and Duration)	Effects	Reference
SPECIES: Rabbit		
20 mg (24 h)	Severe irritation after one drop of pure liquid, symptoms lasted 96 h. Concentrations of 50 and 25 percent ethylhexanol in oil caused irritation but symptoms disappeared 48 and 8 h, respectively, after treatment. 25 percent concentration in oil had no effect.	RTECS 1979; Patty 1982
4165 µg	Severe irritation	RTECS 1979
0.1 mL	Severe irritation	Patty 1982

7.3 Threshold Perception Properties

7.3.1 Odour.

Odour Characteristics: musty, unpleasant to pleasant (Verschueren 1977).

Odour Index: 100 percent recognition, 949 (Verschueren 1977).

Parameter	Media	Concentration	Reference
Absolute Perception Limit	0.075 ppm	Verschueren 1977	
100% Recognition		0.138 ppm	Verschueren 1977
50% Recognition		0.138 ppm	erschueren 1977
20% Detection	In water	0.61 ppm	Verschueren 1977
10% Detection	In water	0.42 ppm	Verschueren 1977
1% Detection	In water	0.12 ppm	Verschueren 1977
0.1% Detection	In water	0.035 ppm	Verschueren 1977
T.O.C. at room temperature	In water	1.3 ppm, range: 0.58 to 20.8 ppm	Verschueren 1977
T.O.C. at room temperature	In water	1.28 ppm	EPA 660/4-75-002

7.3.2 Taste. No data.

7.4 Toxicity Studies

7.4.1 Inhalation.

Exposure Level (and Duration)	Effects	Reference
Acute Exposures		
SPECIES: Rat		
2037 ppm (6 h)	Survived, evidence of irritation and CNS depression	Eastman 1977
235 ppm (6 h)	No deaths, moderate mucous membrane irritation and signs of CNS depression	Verschueren 1977; Patty 1982
227 ppm (6 h)	No deaths, signs of irritation and CNS depression	Eastman 1977

7.4.2 Ingestion.

Exposure Level (and Duration)	Effects	Reference
Acute Exposures		
SPECIES: Human		
0.5 to 5 g/kg	Probable oral lethal dose	TDB (on-line) 1981
SPECIES: Rat		
3.73 g/kg	LD_{50}	Eastman 1977
3.2 to 6.4 g/kg	LD_{50}	Verschueren 1977
2.0 to 3.7 g/kg	LD_{50}, range of a number of experiments	Patty 1982
3200 mg/kg	LD_{50}	GE 1979
SPECIES: Mouse		
3.2 to 6.4 g/kg	LD_{50}, range of a number of experiments	Verschueren 1977; Patty 1982
3200 mg/kg	LD_{LO}	RTECS 1979

7.4.3 Intraperitoneal.

Exposure Level (and Duration)	Effects	Reference
SPECIES: Rat		
800 to 1600 mg/kg	LD_{50}	Eastman 1977
500 to 1000 mg/kg (96 h)	LD_{50}	Dave 1978
SPECIES: Mouse		
780 mg/kg	LD_{50}	Patty 1982
< 400 mg/kg	LD_{50}	Eastman 1977

7.5 Symptoms of Exposure

General symptoms of exposure found in most information sources have not been specifically referenced. Only those of a more specific or unusual nature have their sources indicated.

7.5.1 Inhalation. Exposure to 2-ethylhexanol causes eye and nasal irritation (CCPA 1983). Inhalation of vapours causes irritation of breathing passages, labored respiration and central nervous system depression (Patty 1982).

7.5.2 Ingestion. 2-Ethylhexanol is harmful if swallowed (CHRIS 1978), and slightly toxic when ingested (TDB (on-line) 1981). It may produce symptoms such as noted for inhalation. Long-term or large concentrations may cause liver and kidney damage (Patty 1982).

7.5.3 Skin Contact. Irritating to skin; if spilled on clothing and allowed to remain, may cause smarting and reddening of the skin (CHRIS 1978).

This material is absorbed fairly readily through the skin and can cause sensitization and dermatitis on prolonged or repeated contact (GE 1979).

7.5.4 Eye Contact. Irritating to eyes; vapours cause a slight smarting of the eyes if present in high concentrations. The effect is temporary (CHRIS 1978).

7.5.5 Unspecified Route of Exposure. Anesthesia, nausea, headache, dizziness (CHRIS 1978).

8 CHEMICAL COMPATIBILITY

8.1 Compatibility of 2-Ethylhexanol with Other Chemicals and Chemical Groups

SPECIFIC CHEMICAL OR CHEMICAL GROUP	HEAT GENERATION	FIRE	EXPLOSION	FORMATION OF FLAMMABLE GASES	VIOLENT POLYMERIZATION	DECOMPOSITION	FORMATION OF TOXIC FUMES	FORMATION OF SUBSTANCES OF GREATER TOXICITY	PRESSURIZATION IN CLOSED VESSELS	SOLUBILIZATION	VIOLENT REACTION	NON-HAZARDOUS REACTION	SPECIFICS	REFERENCE
GENERAL														
Heat		•											Moderate fire hazard	Sax 1979
Fire		•											Moderate fire hazard	Sax 1979
CHEMICAL GROUPS														
Oxidizing Agents		•												Sax 1979
Isocyanates			•										Mixture in absence of solvents often explodes violently	NFPA 1978
SPECIFIC CHEMICALS														
Acetaldehyde										•			Condensation reaction could be violent	NFPA 1978
Barium Perchlorate			•										On heating produces perchloric ester which is explosive	NFPA 1978
Chlorine			•										Can produce alkyl hypochlorites which are unstable	NFPA 1978

8.1 Compatibility of 2-Ethylhexanol with Other Chemicals and Chemical Groups (Cont'd)

SPECIFIC CHEMICAL OR CHEMICAL GROUP	HEAT GENERATION	FIRE	EXPLOSION	FORMATION OF FLAMMABLE GASES	VIOLENT POLYMERIZATION	DECOMPOSITION	FORMATION OF TOXIC FUMES	FORMATION OF SUBSTANCES OF GREATER TOXICITY	PRESSURIZATION IN CLOSED VESSELS	SOLUBILIZATION	VIOLENT REACTION	NON-HAZARDOUS REACTION	SPECIFICS	REFERENCE
Ethylene Oxide		•											Can explode	NFPA 1978
Hydrogen Peroxide and Sulphuric Acid		•											Tertiary mixture can explode	NFPA 1978
Hydrochlorous Acid		•											Can produce alkyl hypochlorites which are unstable	NFPA 1978
Nitrogen Tetroxide		•											Can explode	NFPA 1978
Perchloric Acid		•											Can explode, especially if acid is hot	NFPA 1978
Permono-Sulphuric Acid		•											Can explode	NFPA 1978
Triisobutyl Aluminum										•			Reacts violently	NFPA 1978

9 COUNTERMEASURES

9.1 Recommended Handling Procedures

The following procedures have been derived from a literature review. To avoid any deviation from the intended meaning, the wording of the original source has been presented essentially unchanged - in so doing, it is recognized that there may be some discrepancies between different sources of information. It is recognized that countermeasures are dependent on the situation, and thus what may appear to be conflicting information may in fact be correct for different situations. The following procedures should not be considered as Environment Canada's recommendations.

9.1.1 Fire Concerns. 2-Ethylhexanol is a combustible material (NFPA 1978). It is a moderate fire hazard when exposed to heat or flame (GE 1978).

9.1.2 Fire Extinguishing Agents. Use water spray to cool containers involved in a fire (NFPA 1978). Water fog, dry chemical, foam and carbon dioxide can be used as extinguishing media (BASF PSDS 1981).

9.1.3 Spill Actions, Cleanup and Treatment.

9.1.3.1 General. Stop or reduce discharge of material if this can be done without risk. Eliminate all sources of ignition. Avoid skin contact and inhalation (BASF PSDS 1981). Foams can be applied to diminish vapours and reduce fire hazards (CG-D-38-76).

The following absorbent materials have shown possible applicability for vapour suppression and/or containment of 2-ethylhexanol: Carbopol, cellosize and hycar (ICI 1982).

9.1.3.2 Spills on land. Contain if possible, and pick up as much spilled material as possible for recovery or absorb spilled material with sawdust or other absorbent materials and shovel into containers for disposal (GE 1978). Oil spill sorbents are effective for 2-ethylhexanol (MCHSR 1984).

9.1.3.3 Spills in water. Contain using oil spill booms. Oil spill skimmers can be effective for removal (MCHSR 1984).

Recommended sorbent materials to be used in spill situations are: activated carbon, polypropylene fibres, and cellulose fibres (CG-D-38-76). Oil spill sorbents are also effective (MCHSR 1984).

The following treatment processes have shown possible applicability for spill countermeasures:

Process	% Removal (TSA 1980)
Biological	75 - 85
Carbon Adsorption	98

9.1.4 Disposal. Waste 2-ethylhexanol must never be discharged directly into sewers or surface waters. It may be burned in an approved incinerator (GE 1978).

9.1.5 Protective Measures. For entry into a situation where the spilled material and its characteristics are unknown, self-contained breathing apparatus and a totally encapsulated chemical suit should be worn.

If the spilled material is known to be 2-ethylhexanol:

- Safety goggles or face shields, impervious clothing and approved respirators should be worn (GE 1978).
- Eye wash stations and safety showers should be readily available in areas of use and spill situations (GE 1978).

9.1.6 Storage Precautions. Store in a cool, dry place away from heat and sources of ignition (GE 1978).

10 PREVIOUS SPILL EXPERIENCE

10.1 Train Derailment (Personal Communication with EPS 1982; SPE 1979)

Six tank cars, three containing 2-ethylhexanol, two containing propane and one containing resin, overturned near a creek in an urban area. The water from the creek flows into a river which drains into a reservoir approximately 8 or 9 km from the accident site. This reservoir supplies potable water to a nearby community.

Residents in the area were evacuated because of the potential for propane gas explosions. Firefighters arrived at the spill site and immediately applied a water spray to the propane tank cars, keeping them cool to prevent bursting. Firefighters wore self-contained breathing apparatus for personal protection.

Response personnel arrived at the site a few hours later and found that the liquid being spilled in the creek was 2-ethylhexanol. One of the tank cars containing 2-ethylhexanol had a puncture, which was quickly repaired by hammering in pieces of 2 x 4 until the leak stopped. The second car had its ball valve broken off, spilling most of its contents. The third car did not suffer any damage.

Several containment measures were undertaken in the river to prevent the spilled material from reaching the reservoir. An earthen dyke was built at a bridge near the spill site and absorbent materials applied to remove the 2-ethylhexanol. A short distance downstream, oil booms and bales of hay were deployed to further contain the spilled material. A nearby community, after being notified of the 2-ethylhexanol spill, built a large earthen dyke across the river approximately 3 km downstream from the site. Later that day, modifications to the dyke had to be made to prevent possible problems resulting from greater flows after a rainfall. Pipes were inserted near the bottom of the dyke to allow some drainage and thus reduce the pressure at the front of the dyke.

On the next day, transfer of the contents from the derailed cars into tank trucks proceeded. The spilled product, contained above the dykes, was pumped out and shipped to a nearby waste management facility for incineration. Dead fish were noted at the large dyke and later that day at the confluence of the reservoir. This prompted the placement of absorbent oil booms at a bridge downstream from the large dyke. The odours of 2-ethylhexanol were noted up to 8 km from the spill site. Water samples were taken along the river and in the reservoir. The analyses revealed that the concentrations of 2-ethylhexanol were over 300 mg/L above the dyke and 150 mg/L below it. The concentration decreased to approximately 20 to 30 mg/L at the confluence of the

reservoir, where dead fish were noted, and down to 10 mg/L at a further distance into the reservoir.

Dissolved oxygen readings indicated that the oxygen level in the lake was sufficient for fish to survive. It was concluded that the main reason for the fish kill was the presence of 2-ethylhexanol in the water. The vegetation, where the spilled material had contacted the edge of water and ground, was also found to be affected after 24 hours. Very low concentrations of 2-ethylhexanol were noted at the pumping station for potable water.

It was estimated (by response personnel) that approximately 120 000 L of 2-ethylhexanol had been spilled into the river. Approximately 365 000 L of water contaminated with 2-ethylhexanol were removed from the river and shipped away for incineration. During cleanup, dead fish were picked up continually to prevent decaying fish from causing bacteriological effects in the water. Approximately 7 tonnes of dead fish were removed from the river and reservoir. Even though very low concentrations of 2-ethylhexanol were noted at the pumping station, sensitive individuals could detect the odour, especially in warm water.

11 ANALYTICAL METHODS

The general approach adopted for each of the Priority Chemicals was as follows.

Methods have been documented here for the analysis of samples from air, water and soil in a normally equipped chemical laboratory remote from the spill site. Customary sources of standard or recommended analytical methods were consulted, and outlines are presented for each chemical. These sources included publications of the U.S. National Institute for Occupational Safety and Health (NIOSH), the U.S. Environmental Protection Agency (EPA), the American Water Works Association (AWWA), the American Society for Testing and Materials (ASTM), and the American National Standards Institute (ANSI).

If the standard or recommended methods were judged to be reliable and specific enough for the analysis of environmental and materials samples from spill sites, and if they do not require highly specialized laboratory equipment, no additional methods were sought.

If especially simple, reliable tests (e.g., commonly used industrial methods) were found, they have been presented as well.

11.1 Quantitative Method for the Detection of 2-Ethylhexanol in Air

11.1.1 Gas Chromatography (NIOSH 1977). Although this NIOSH method is for cyclohexanol, it may be used for 2-ethylhexanol. A range of 123 to 494 mg/m^3 (23 to 93 ppm) of 2-ethylhexanol in air may be determined by adsorption on charcoal, desorption with carbon disulphide, followed by gas chromatographic analysis.

A known volume of air is drawn through a glass charcoal tube. A 10 L sample is recommended at a flow rate of 200 cc/min. The charcoal tube is 7 cm long, 6 mm O.D. and 4 mm I.D. It contains two sections of 20/40 mesh activated charcoal separated by a 2 mm portion of urethane foam. The front section contains 100 mg of charcoal whereas the back-up section contains 50 mg of charcoal. A 3 mm portion of urethane foam is placed between the outlet end of the tube and the back-up section. A plug of silylated glass wool is placed in front of the absorbing section.

Before sampling, the ends of the charcoal tube are broken and the back-up section positioned nearest the pump and the tube held in a vertical position. A sample size of 10 L is recommended at a flow rate of 0.2 L/s or less. After sampling, the tube is stoppered. For analysis, the tube is scored with a file in front of the first section and

broken. The charcoal in the first section is then transferred into a 2 mL glass vial with a Teflon cap. The back-up section is placed in a separate 2 mL capacity glass vial. A 1.0 mL volume of carbon disulphide (chromatographic quality containing 0.2 percent solution of internal standard, 2-propanol, may be used) is added to the sample vial and desorption is allowed to continue for 30 minutes. Occasional agitation is recommended. A 5 µL aliquot of sample is injected into a suitable gas chromatograph equipped with a flame ionization detector. The solvent flush injection technique is recommended. The back-up section is also analyzed by the same method. If a significant reading is obtained on this portion, breakthrough has occurred and the sample size too great.

Typical gas chromatograph operating conditions are: nitrogen carrier gas flow at 30 mL/min (80 psig), hydrogen gas flow to detector at 30 mL/min (50 psig), air flow to detector at 300 mL/min (50 psig), injector temperature at 200°C, detector temperature at 300°C, and column temperature at 120°C. The column is 10 ft. x 1/8 in. stainless steel packed with 10 percent FFAP on 80/100 mesh Chromosorb W-AW.

The 2-ethylhexanol is determined using a suitable electronic integrator to measure peak area in conjunction with a standard curve.

11.2 Qualitative Method for the Detection of 2-Ethylhexanol in Air

The sample is collected as in Section 11.1.1 and desorbed. Acetyl chloride (three to four drops) is placed in a dry test tube and the fumes resulting from the reaction with atmospheric moisture are allowed to dissipate. The sample is added dropwise to the test tube until a total of three drops have been added. A positive indication is given by: a vigorous reaction, the mixture boils spontaneously, heat of reaction, the mixture becomes warm, hydrogen chloride gas is evolved. A further step may be followed. The mixture is cooled in ice and several drops of water are added. The mixture is shaken then made alkaline with dilute sodium hydroxide solution. A pleasant fruity smell indicates a volatile ester and thus the presence of an alcohol before the reaction (Owen 1969).

11.3 Quantitative Method for the Detection of 2-Ethylhexanol in Water

11.3.1 Gas Chromatography (ASTM 1983). A wide range of 2-ethylhexanol concentrations may be determined using direct aqueous injection into a gas chromatograph equipped with a flame ionization detector.

A minimum of 2 L of representative sample is collected in a clean, glass bottle having a screw cap lined with aluminum foil or TFE-fluorocarbon. A 2 to 5 µL sample is injected into a gas chromatograph equipped with a flame ionization detector. Kovats

index or retention time is used to identify the compound; the area and the peak may be used to quantitate the compound by direct comparison with standard responses.

Typical gas chromatograph operating conditions are: a flame ionization detector, helium carrier gas flow at 45 mL/min, injector temperature 165 to 260°C, detector temperature at 250°C, column temperature at 50-250°C at 8°C/min. The column is 20 ft. x 1/8 in. O.D. stainless steel packed with Carbowax 20M (5 percent) 80/100 A.W, Chromosorb W.

11.4 Quantitative Method for the Detection of 2-Ethylhexanol in Soil

11.4.1 Gas Chromatography (ASTM 1983; NIOSH 1977). A wide range of 2-ethylhexanol concentrations in the extracting solution may be detected using a flame ionization detector.

Approximately 20 g of soil, accurately weighed, are collected in a glass jar and dried by the addition of magnesium sulphate.

A suitable amount of Freon• 113 (1,1,2-trichloro-1,2,2-trifluoroethane) is used to extract the 2-ethylhexanol from the soil. The Freon• is distilled from the soil on a water bath at 70°C. Air is drawn through the containing flask for the final minute to remove all traces of Freon•. The residue is dissolved in a suitable amount of carbon disulphide and an aliquot is injected directly into a gas chromatograph equipped with a flame ionization detector. Typical gas chromatograph conditions are: a 10 ft. x 1/8 inch stainless steel column packed with 10 percent FFAP on 80/100 mesh acid washed DMCS Chromosorb W, injector temperature at 195°C, column temperature at 85°C, detector temperature at 250°C, nitrogen carrier gas flow at 50 mL/min, hydrogen gas flow at 65 mL/min, air flow at 500 mL/min. Retention time is used to identify the compound and peak areas are used to quantitate. Standard samples should be processed in the identical manner to the above to ensure all losses are compensated for.

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EnviroTIPS

Common Abbreviations

BOD	biological oxygen demand
b.p.	boiling point
CC	closed cup
cm	centimetre
CMD	count median diameter
COD	chemical oxygen demand
conc	concentration
c.t.	critical temperature
eV	electron volt
g	gram
ha	hectare
Hg	mercury
IDLH	immediately dangerous to life and health
Imp. gal.	imperial gallon
in.	inch
J	joule
kg	kilogram
kJ	kilojoule
km	kilometre
kPa	kilopascal
kt	kilotonne
L	litre
lb.	pound
LC_{50}	lethal concentration fifty
LC_{LO}	lethal concentration low
LD_{50}	lethal dose fifty
LD_{LO}	lethal dose low
LEL	lower explosive limit
LFL	lower flammability limit
m	metre
m	meta
M	molar
MAC	maximum acceptable concentration
max	maximum
mg	milligram
MIC	maximum immission concentration
min	minute or minimum
mm	millimetre
µg	microgram
µm	micrometre
°Be	degrees Baumé (density)
MMAD	mass median aerodynamic diameter
MMD	mass median diameter
m.p.	melting point
MW	molecular weight
N	newton
NAS	National Academy of Sciences
NFPA	National Fire Protection Association
NIOSH	National Institute for Occupational Safety and Health
nm	nanometre
o	ortho
OC	open cup
p	para
P_c	critical pressure
PEL	permissible exposure level
pH	measure of acidity/ alkalinity
ppb	parts per billion
ppm	parts per million
P_s	standard pressure
psi	pounds per square inch
s	second
STEL	short-term exposure limit
STIL	short-term inhalation limit
T_c	critical temperature
TC_{LO}	toxic concentration low
Td	decomposition temperature
TD_{LO}	toxic dose low
TL_m	median tolerance limit
TLV	Threshold Limit Value
Ts	standard temperature
TWA	time weighted average
UEL	upper explosive limit
UFL	upper flammability limit
VMD	volume mean diameter
v/v	volume per volume
w/w	weight per weight